Benzoic acid, undecyl ester

Other names: undecyl benzoate
Inchi: InChI=1S/C18H28O2/c1-2-3-4-5-6-7-8-9-13-16-20-18(19)17-14-11-10-12-15-17/h10-12,1
InchiKey: YEHGKFOTJWYCBN-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 276.41
CAS: 6316-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-20.83	kJ/mol	Joback Method
hf	-423.12	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.374		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2063.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2064.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2076.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2583.00		NIST Webbook

ripol	2601.00		NIST Webbook
ripol	2574.00		NIST Webbook
ripol	2594.00		NIST Webbook
ripol	2578.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2576.00		NIST Webbook
ripol	2601.00		NIST Webbook
ripol	2578.00		NIST Webbook
tb	714.21	K	Joback Method
tc	906.19	K	Joback Method
tf	391.20	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.91	J/mol×K	714.21	Joback Method
cpg	790.14	J/mol×K	874.20	Joback Method
cpg	776.16	J/mol×K	842.20	Joback Method
cpg	761.28	J/mol×K	810.20	Joback Method
cpg	745.47	J/mol×K	778.20	Joback Method
cpg	728.69	J/mol×K	746.21	Joback Method
cpg	803.25	J/mol×K	906.19	Joback Method
dvisc	0.0000958	Pa×s	714.21	Joback Method
dvisc	0.0001261	Pa×s	660.38	Joback Method
dvisc	0.0001743	Pa×s	606.54	Joback Method
dvisc	0.0002566	Pa×s	552.70	Joback Method
dvisc	0.0004105	Pa×s	498.87	Joback Method
dvisc	0.0007359	Pa×s	445.03	Joback Method
dvisc	0.0015490	Pa×s	391.20	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6316309&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume