Isophthalic acid, heptadecyl 3-methylpentyl-2 ester

Other names: Isophthalic acid, heptadecyl 3-methylbut-2-yl ester
Inchi: InChI=1S/C31H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-34-30(32)28-22-
InchiKey: YHMYHRUHBKTLMM-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)CC)c1
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-159.80	kJ/mol	Joback Method
hf	-958.27	kJ/mol	Joback Method
hfus	68.23	kJ/mol	Joback Method
hvap	105.07	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.306		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	703.59	kPa	Joback Method
rinpol	3569.00		NIST Webbook
tb	1092.04	K	Joback Method
tc	1353.20	K	Joback Method
tf	592.39	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.07	J/mol×K	1092.04	Joback Method
cpg	1579.98	J/mol×K	1135.57	Joback Method
cpg	1596.64	J/mol×K	1179.09	Joback Method
cpg	1611.18	J/mol×K	1222.62	Joback Method
cpg	1623.70	J/mol×K	1266.15	Joback Method
cpg	1634.32	J/mol×K	1309.67	Joback Method
cpg	1643.16	J/mol×K	1353.20	Joback Method
dvisc	0.0001919	Pa×s	592.39	Joback Method

dvisc	0.0000831	Pa×s	675.67	Joback Method
dvisc	0.0000432	Pa×s	758.94	Joback Method
dvisc	0.0000256	Pa×s	842.22	Joback Method
dvisc	0.0000166	Pa×s	925.49	Joback Method
dvisc	0.0000116	Pa×s	1008.76	Joback Method
dvisc	0.0000086	Pa×s	1092.04	Joback Method

Sources

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=U356162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume