o-Toluic acid, 2-naphthyl ester

Other names: o-Toluylic acid, 2-naphthyl ester
Inchi: InChI=1S/C18H14O2/c1-13-6-2-5-9-17(13)18(19)20-16-11-10-14-7-3-4-8-15(14)12-16/h2
InchiKey: LJIQFSNCVVGXSR-UHFFFAOYSA-N
Formula: C18H14O2
SMILES: Cc1ccccc1C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	178.97	kJ/mol	Joback Method
hf	-18.46	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.367		Crippen Method
mcvol	204.940	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	769.83	K	Joback Method
tc	1021.87	K	Joback Method
tf	475.36	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.08	J/mol×K	769.83	Joback Method
cpg	569.74	J/mol×K	811.84	Joback Method
cpg	583.16	J/mol×K	853.84	Joback Method
cpg	595.43	J/mol×K	895.85	Joback Method
cpg	606.66	J/mol×K	937.86	Joback Method
cpg	616.95	J/mol×K	979.87	Joback Method
cpg	626.39	J/mol×K	1021.87	Joback Method

dvisc	0.0009517	Pa×s	475.36	Joback Method
dvisc	0.0006369	Pa×s	524.44	Joback Method
dvisc	0.0004565	Pa×s	573.52	Joback Method
dvisc	0.0003449	Pa×s	622.60	Joback Method
dvisc	0.0002714	Pa×s	671.67	Joback Method
dvisc	0.0002207	Pa×s	720.75	Joback Method
dvisc	0.0001843	Pa×s	769.83	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=U307461&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume