Succinic acid, 8-chlorooctyl 2-naphthyl ester

Inchi: InChI=1S/C22H27ClO4/c23-15-7-3-1-2-4-8-16-26-21(24)13-14-22(25)27-20-12-11-18-9-5
InchiKey: OQTZKIJVHFPZGI-UHFFFAOYSA-N
Formula: C22H27ClO4
SMILES: O=C(CCC(=O)Oc1ccc2ccccc2c1)OCCCCCCCCCl
Mol. weight [g/mol]: 390.90

Physical Properties

Property code	Value	Unit	Source
gf	-135.98	kJ/mol	Joback Method
hf	-586.62	kJ/mol	Joback Method
hfus	53.18	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.648		Crippen Method
mcvol	304.740	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
tb	943.41	K	Joback Method
tc	1162.60	K	Joback Method
tf	583.58	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.34	J/mol×K	943.41	Joback Method
cpg	958.17	J/mol×K	979.94	Joback Method
cpg	970.90	J/mol×K	1016.47	Joback Method
cpg	982.62	J/mol×K	1053.01	Joback Method
cpg	993.37	J/mol×K	1089.54	Joback Method
cpg	1003.23	J/mol×K	1126.07	Joback Method
cpg	1012.25	J/mol×K	1162.60	Joback Method
dvisc	0.0005052	Pa×s	583.58	Joback Method

dvisc	0.0003142	Pa×s	643.55	Joback Method
dvisc	0.0002119	Pa×s	703.52	Joback Method
dvisc	0.0001520	Pa×s	763.50	Joback Method
dvisc	0.0001144	Pa×s	823.47	Joback Method
dvisc	0.0000896	Pa×s	883.44	Joback Method
dvisc	0.0000723	Pa×s	943.41	Joback Method

Sources

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=U389842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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