

Succinic acid, 2-naphthylmethyl tridecyl ester

Inchi:	InChI=1S/C28H40O4/c1-2-3-4-5-6-7-8-9-10-11-14-21-31-27(29)19-20-28(30)32-23-24-17
InchiKey:	BWROIDUVMIAAND-UHFFFAOYSA-N
Formula:	C28H40O4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	440.61

Physical Properties

Property code	Value	Unit	Source
gf	-73.53	kJ/mol	Joback Method
hf	-694.72	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.517		Crippen Method
mvol	377.040	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3426.00		NIST Webbook
rinpol	3426.00		NIST Webbook
tb	1043.26	K	Joback Method
tc	1278.22	K	Joback Method
tf	621.28	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.64	J/molxK	1043.26	Joback Method
cpg	1303.26	J/molxK	1082.42	Joback Method
cpg	1318.52	J/molxK	1121.58	Joback Method
cpg	1332.52	J/molxK	1160.74	Joback Method
cpg	1345.35	J/molxK	1199.90	Joback Method
cpg	1357.12	J/molxK	1239.06	Joback Method
cpg	1367.92	J/molxK	1278.22	Joback Method
dvisc	0.0003202	Paxs	621.28	Joback Method

dvisc	0.0001845	Paxs	691.61	Joback Method
dvisc	0.0001177	Paxs	761.94	Joback Method
dvisc	0.0000810	Paxs	832.27	Joback Method
dvisc	0.0000591	Paxs	902.60	Joback Method
dvisc	0.0000451	Paxs	972.93	Joback Method
dvisc	0.0000357	Paxs	1043.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U389992&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

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