

Succinic acid, naphth-2-ylmethyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C23H30O4/c1-17(14-23(2,3)4)15-26-21(24)11-12-22(25)27-16-18-9-10-19-7-5
InchiKey:	RDUJXPXIIGWVAFY-UHFFFAOYSA-N
Formula:	C23H30O4
SMILES:	CC(COC(=O)CCC(=O)OCc1ccc2ccccc2c1)CC(C)(C)C
Mol. weight [g/mol]:	370.48

Physical Properties

Property code	Value	Unit	Source
gf	-115.23	kJ/mol	Joback Method
hf	-605.55	kJ/mol	Joback Method
hfus	40.63	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.279		Crippen Method
mvol	306.590	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2761.00		NIST Webbook
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tb	925.19	K	Joback Method
tc	1146.34	K	Joback Method
tf	552.35	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.53	J/molxK	925.19	Joback Method
cpg	995.93	J/molxK	962.05	Joback Method
cpg	1010.21	J/molxK	998.91	Joback Method
cpg	1023.45	J/molxK	1035.76	Joback Method
cpg	1035.74	J/molxK	1072.62	Joback Method
cpg	1047.17	J/molxK	1109.48	Joback Method
cpg	1057.83	J/molxK	1146.34	Joback Method
dvisc	0.0005184	Paxs	552.35	Joback Method

dvisc	0.0002898	Paxs	614.49	Joback Method
dvisc	0.0001803	Paxs	676.63	Joback Method
dvisc	0.0001215	Paxs	738.77	Joback Method
dvisc	0.0000870	Paxs	800.91	Joback Method
dvisc	0.0000654	Paxs	863.05	Joback Method
dvisc	0.0000511	Paxs	925.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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