

Succinic acid, naphth-2-ylmethyl 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C23H22O4/c1-16-6-5-9-21(17(16)2)27-23(25)13-12-22(24)26-15-18-10-11-19-
InchiKey:	MQIFXZXDEVMGAR-UHFFFAOYSA-N
Formula:	C23H22O4
SMILES:	<chem>Cc1cccc(OC(=O)CCC(=O)OCc2ccc3ccccc3c2)c1C</chem>
Mol. weight [g/mol]:	362.42

Physical Properties

Property code	Value	Unit	Source
gf	-22.48	kJ/mol	Joback Method
hf	-377.93	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	93.28	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	4.886		Crippen Method
mvol	282.830	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	3219.00		NIST Webbook
rinpol	3219.00		NIST Webbook
tb	965.50	K	Joback Method
tc	1203.33	K	Joback Method
tf	616.39	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.80	J/molxK	965.50	Joback Method
cpg	885.59	J/molxK	1005.14	Joback Method
cpg	897.17	J/molxK	1044.78	Joback Method
cpg	907.61	J/molxK	1084.41	Joback Method
cpg	916.97	J/molxK	1124.05	Joback Method
cpg	925.34	J/molxK	1163.69	Joback Method
cpg	932.78	J/molxK	1203.33	Joback Method
dvisc	0.0004197	Paxs	616.39	Joback Method

dvisc	0.0002826	Paxs	674.58	Joback Method
dvisc	0.0002025	Paxs	732.76	Joback Method
dvisc	0.0001525	Paxs	790.95	Joback Method
dvisc	0.0001193	Paxs	849.13	Joback Method
dvisc	0.0000964	Paxs	907.32	Joback Method
dvisc	0.0000799	Paxs	965.50	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=U390034&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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