

Succinic acid, naphth-2-ylmethyl neopentyl ester

Inchi:	InChI=1S/C20H24O4/c1-20(2,3)14-24-19(22)11-10-18(21)23-13-15-8-9-16-6-4-5-7-17(16)
InchiKey:	TVPOVAMESVIII-UHFFFAOYSA-N
Formula:	C20H24O4
SMILES:	CC(C)(C)COC(=O)CCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	-138.05	kJ/mol	Joback Method
hf	-538.35	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.253		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	856.99	K	Joback Method
tc	1078.11	K	Joback Method
tf	533.54	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/mol×K	856.99	Joback Method
cpg	867.50	J/mol×K	1041.25	Joback Method
cpg	856.66	J/mol×K	1004.40	Joback Method
cpg	844.95	J/mol×K	967.55	Joback Method
cpg	832.32	J/mol×K	930.70	Joback Method
cpg	818.67	J/mol×K	893.84	Joback Method
cpg	877.56	J/mol×K	1078.11	Joback Method
dvisc	0.0000851	Paxs	856.99	Joback Method

dvisc	0.0001064	Paxs	803.08	Joback Method
dvisc	0.0001374	Paxs	749.17	Joback Method
dvisc	0.0001847	Paxs	695.26	Joback Method
dvisc	0.0002608	Paxs	641.36	Joback Method
dvisc	0.0003924	Paxs	587.45	Joback Method
dvisc	0.0006413	Paxs	533.54	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=U389592&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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