

Succinic acid, cyclohexylmethyl 2-naphthylmethyl ester

Inchi: InChI=1S/C22H26O4/c23-21(25-15-17-6-2-1-3-7-17)12-13-22(24)26-16-18-10-11-19-8-4
InchiKey: MITSERAVLBMHHZ-UHFFFAOYSA-N
Formula: C22H26O4
SMILES: O=C(CCC(=O)OCC1CCCCC1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 354.44

Physical Properties

Property code	Value	Unit	Source
gf	-99.60	kJ/mol	Joback Method
hf	-516.56	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	87.89	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.787		Crippen Method
mvol	281.640	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	3036.00		NIST Webbook
rinpol	3036.00		NIST Webbook
tb	925.53	K	Joback Method
tc	1158.89	K	Joback Method
tf	561.04	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.94	J/molxK	925.53	Joback Method
cpg	929.30	J/molxK	964.42	Joback Method
cpg	943.23	J/molxK	1003.32	Joback Method
cpg	955.79	J/molxK	1042.21	Joback Method
cpg	967.06	J/molxK	1081.10	Joback Method
cpg	977.11	J/molxK	1120.00	Joback Method
cpg	986.04	J/molxK	1158.89	Joback Method
dvisc	0.0006764	Paxs	561.04	Joback Method

dvisc	0.0004063	Paxs	621.79	Joback Method
dvisc	0.0002672	Paxs	682.54	Joback Method
dvisc	0.0001882	Paxs	743.28	Joback Method
dvisc	0.0001398	Paxs	804.03	Joback Method
dvisc	0.0001082	Paxs	864.78	Joback Method
dvisc	0.0000867	Paxs	925.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390005&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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