

Succinic acid, cyclohexylmethyl 2-naphthyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C21H24O4/c22-20(24-15-16-6-2-1-3-7-16)12-13-21(23)25-19-11-10-17-8-4-5-9

YTLYNEHVIXVEHX-UHFFFAOYSA-N

C21H24O4

O=C(CCC(=O)Oc1ccc2ccccc2c1)OCC1CCCCC1

340.41

Physical Properties

Property code	Value	Unit	Source
gf	-108.02	kJ/mol	Joback Method
hf	-495.92	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	85.66	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.649		Crippen Method
mcvol	267.550	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	902.65	K	Joback Method
tc	1138.01	K	Joback Method
tf	549.77	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.93	J/mol×K	902.65	Joback Method
cpg	870.33	J/mol×K	941.88	Joback Method
cpg	884.28	J/mol×K	981.10	Joback Method
cpg	896.86	J/mol×K	1020.33	Joback Method
cpg	908.14	J/mol×K	1059.56	Joback Method
cpg	918.19	J/mol×K	1098.78	Joback Method
cpg	927.10	J/mol×K	1138.01	Joback Method
dvisc	0.0007434	Pa×s	549.77	Joback Method

dvisc	0.0004518	Pa×s	608.58	Joback Method
dvisc	0.0002997	Pa×s	667.40	Joback Method
dvisc	0.0002125	Pa×s	726.21	Joback Method
dvisc	0.0001587	Pa×s	785.02	Joback Method
dvisc	0.0001234	Pa×s	843.84	Joback Method
dvisc	0.0000991	Pa×s	902.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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