

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

Inchi:	InChI=1S/C21H26O4/c1-3-16(2)12-13-24-20(22)10-11-21(23)25-15-17-8-9-18-6-4-5-7-19
InchiKey:	JRUKGIZWBZCKJX-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CCC(C)CCOC(=O)CCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-134.91	kJ/mol	Joback Method
hf	-555.52	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.643		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2818.00		NIST Webbook
rinpol	2818.00		NIST Webbook
tb	882.66	K	Joback Method
tc	1098.28	K	Joback Method
tf	527.39	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.57	J/molxK	882.66	Joback Method
cpg	876.41	J/molxK	918.60	Joback Method
cpg	890.13	J/molxK	954.53	Joback Method
cpg	902.78	J/molxK	990.47	Joback Method
cpg	914.42	J/molxK	1026.41	Joback Method
cpg	925.10	J/molxK	1062.35	Joback Method
cpg	934.88	J/molxK	1098.28	Joback Method
dvisc	0.0007083	Paxs	527.39	Joback Method

dvisc	0.0004187	Paxs	586.60	Joback Method
dvisc	0.0002725	Paxs	645.81	Joback Method
dvisc	0.0001907	Paxs	705.03	Joback Method
dvisc	0.0001410	Paxs	764.24	Joback Method
dvisc	0.0001089	Paxs	823.45	Joback Method
dvisc	0.0000871	Paxs	882.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390658&Units=SI
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

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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