

Succinic acid, 8-chlorooctyl 2-naphthylmethyl ester

Inchi:	InChI=1S/C23H29ClO4/c24-15-7-3-1-2-4-8-16-27-22(25)13-14-23(26)28-18-19-11-12-20
InchiKey:	LLEWPQILPVATSY-UHFFFAOYSA-N
Formula:	C23H29ClO4
SMILES:	O=C(CCC(=O)OCc1ccc2ccccc2c1)OCCCCCCCCI
Mol. weight [g/mol]:	404.93

Physical Properties

Property code	Value	Unit	Source
gf	-127.56	kJ/mol	Joback Method
hf	-607.26	kJ/mol	Joback Method
hfus	55.77	kJ/mol	Joback Method
hvap	94.07	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.786		Crippen Method
mvol	318.830	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	966.29	K	Joback Method
tc	1187.28	K	Joback Method
tf	594.85	K	Joback Method
vc	1.234	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.96	J/molxK	966.29	Joback Method
cpg	1063.84	J/molxK	1150.45	Joback Method
cpg	1053.82	J/molxK	1113.62	Joback Method
cpg	1042.89	J/molxK	1076.79	Joback Method
cpg	1030.98	J/molxK	1039.95	Joback Method
cpg	1018.03	J/molxK	1003.12	Joback Method
cpg	1073.01	J/molxK	1187.28	Joback Method
dvisc	0.0000628	Paxs	966.29	Joback Method

dvisc	0.0000780	Paxs	904.38	Joback Method
dvisc	0.0001001	Paxs	842.48	Joback Method
dvisc	0.0001337	Paxs	780.57	Joback Method
dvisc	0.0001876	Paxs	718.66	Joback Method
dvisc	0.0002805	Paxs	656.76	Joback Method
dvisc	0.0004562	Paxs	594.85	Joback Method

Sources

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=U390009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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