

Sebacic acid, 8-chlorooctyl propyl ester

Inchi:	InChI=1S/C21H39ClO4/c1-2-18-25-20(23)15-11-7-3-4-8-12-16-21(24)26-19-14-10-6-5-9
InchiKey:	JQFCWZUAHHYYQG-UHFFFAOYSA-N
Formula:	C21H39ClO4
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	390.99

Physical Properties

Property code	Value	Unit	Source
gf	-353.83	kJ/mol	Joback Method
hf	-982.11	kJ/mol	Joback Method
hfus	59.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.183		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinsol	2791.00		NIST Webbook
tb	869.89	K	Joback Method
tc	1065.07	K	Joback Method
tf	500.67	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.81	J/molxK	869.89	Joback Method
cpg	1079.61	J/molxK	902.42	Joback Method
cpg	1096.23	J/molxK	934.95	Joback Method
cpg	1111.70	J/molxK	967.48	Joback Method
cpg	1126.05	J/molxK	1000.01	Joback Method
cpg	1139.30	J/molxK	1032.54	Joback Method
cpg	1151.48	J/molxK	1065.07	Joback Method
dvisc	0.0005888	Paxs	500.67	Joback Method
dvisc	0.0002928	Paxs	562.21	Joback Method

dvisc	0.0001671	Paxs	623.74	Joback Method
dvisc	0.0001055	Paxs	685.28	Joback Method
dvisc	0.0000718	Paxs	746.82	Joback Method
dvisc	0.0000519	Paxs	808.35	Joback Method
dvisc	0.0000392	Paxs	869.89	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=U355528&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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