Sebacic acid, 8-chlorooctyl hexyl ester

Inchi: InChI=1S/C24H45ClO4/c1-2-3-4-16-21-28-23(26)18-13-9-5-6-10-14-19-24(27)29-22-17-1
InchiKey: QMOGOTCAENXODL-UHFFFAOYSA-N
Formula: C24H45ClO4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 433.06

Physical Properties

Property code	Value	Unit	Source
gf	-328.57	kJ/mol	Joback Method
hf	-1044.03	kJ/mol	Joback Method
hfus	67.69	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.353		Crippen Method
mcvol	376.140	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3108.00		NIST Webbook
rinpol	3108.00		NIST Webbook
tb	938.53	K	Joback Method
tc	1152.36	K	Joback Method
tf	534.48	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.50	J/mol×K	938.53	Joback Method
cpg	1267.78	J/mol×K	974.17	Joback Method
cpg	1285.57	J/mol×K	1009.81	Joback Method
cpg	1301.90	J/mol×K	1045.44	Joback Method
cpg	1316.83	J/mol×K	1081.08	Joback Method
cpg	1330.39	J/mol×K	1116.72	Joback Method
cpg	1342.63	J/mol×K	1152.36	Joback Method
dvisc	0.0004067	Pa×s	534.48	Joback Method

dvisc	0.0001963	Pa×s	601.82	Joback Method
dvisc	0.0001097	Pa×s	669.16	Joback Method
dvisc	0.0000682	Pa×s	736.50	Joback Method
dvisc	0.0000459	Pa×s	803.85	Joback Method
dvisc	0.0000329	Pa×s	871.19	Joback Method
dvisc	0.0000247	Pa×s	938.53	Joback Method

Sources

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=U355533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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