Sebacic acid, hexyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C18H31Cl3O4/c1-2-3-4-11-14-24-16(22)12-9-7-5-6-8-10-13-17(23)25-15-18(19
InchiKey: PDWZXDNMAHLCCS-UHFFFAOYSA-N
Formula: C18H31Cl3O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 417.80

Physical Properties

Property code	Value	Unit	Source
gf	-400.11	kJ/mol	Joback Method
hf	-960.42	kJ/mol	Joback Method
hfus	53.13	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.144		Crippen Method
mcvol	316.080	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
tb	872.88	K	Joback Method
tc	1072.77	K	Joback Method
tf	529.12	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.85	J/mol×K	872.88	Joback Method
cpg	1002.17	J/mol×K	1039.45	Joback Method
cpg	991.37	J/mol×K	1006.14	Joback Method
cpg	979.68	J/mol×K	972.82	Joback Method
cpg	967.05	J/mol×K	939.51	Joback Method
cpg	953.46	J/mol×K	906.19	Joback Method
cpg	1012.11	J/mol×K	1072.77	Joback Method
dvisc	0.0000345	Pa×s	872.88	Joback Method

dvisc	0.0000458	Pa×s	815.59	Joback Method
dvisc	0.0000633	Pa×s	758.29	Joback Method
dvisc	0.0000922	Pa×s	701.00	Joback Method
dvisc	0.0001438	Pa×s	643.71	Joback Method
dvisc	0.0002444	Pa×s	586.41	Joback Method
dvisc	0.0004661	Pa×s	529.12	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=U355314&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