Sebacic acid, isobutyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C16H27Cl3O4/c1-13(2)11-22-14(20)9-7-5-3-4-6-8-10-15(21)23-12-16(17,18)19

InchiKey: AAKADIBGIUAMMB-UHFFFAOYSA-N

Formula: C16H27Cl3O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 389.74

Physical Properties

Property code	Value	Unit	Source
gf	-419.39	kJ/mol	Joback Method
hf	-924.42	kJ/mol	Joback Method
hfus	44.42	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.220		Crippen Method
mcvol	287.900	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2373.00		NIST Webbook
rinpol	2373.00		NIST Webbook
tb	826.68	K	Joback Method
tc	1024.91	K	Joback Method
tf	491.58	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.25	J/mol×K	826.68	Joback Method
cpg	837.28	J/mol×K	859.72	Joback Method
cpg	850.36	J/mol×K	892.76	Joback Method
cpg	862.52	J/mol×K	925.80	Joback Method
cpg	873.79	J/mol×K	958.84	Joback Method
cpg	884.21	J/mol×K	991.87	Joback Method
cpg	893.80	J/mol×K	1024.91	Joback Method
dvisc	0.0006905	Pa×s	491.58	Joback Method

dvisc	0.0003448	Pa×s	547.43	Joback Method
dvisc	0.0001958	Pa×s	603.28	Joback Method
dvisc	0.0001224	Pa×s	659.13	Joback Method
dvisc	0.0000823	Pa×s	714.98	Joback Method
dvisc	0.0000587	Pa×s	770.83	Joback Method
dvisc	0.0000437	Pa×s	826.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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