Sebacic acid, butyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C16H27Cl3O4/c1-2-3-12-22-14(20)10-8-6-4-5-7-9-11-15(21)23-13-16(17,18)19
InchiKey: BRXPFIRGSPDVTJ-UHFFFAOYSA-N
Formula: C16H27Cl3O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 389.74

Physical Properties

Property code	Value	Unit	Source
gf	-416.95	kJ/mol	Joback Method
hf	-919.14	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	81.38	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.364		Crippen Method
mcvol	287.900	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	827.12	K	Joback Method
tc	1023.65	K	Joback Method
tf	506.58	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.70	J/mol×K	827.12	Joback Method
cpg	836.62	J/mol×K	859.88	Joback Method
cpg	849.62	J/mol×K	892.63	Joback Method
cpg	861.72	J/mol×K	925.39	Joback Method
cpg	872.95	J/mol×K	958.14	Joback Method
cpg	883.35	J/mol×K	990.90	Joback Method
cpg	892.96	J/mol×K	1023.65	Joback Method
dvisc	0.0005990	Pa×s	506.58	Joback Method

dvisc	0.0003213	Pa×s	560.00	Joback Method
dvisc	0.0001921	Pa×s	613.43	Joback Method
dvisc	0.0001247	Pa×s	666.85	Joback Method
dvisc	0.0000863	Pa×s	720.27	Joback Method
dvisc	0.0000628	Pa×s	773.70	Joback Method
dvisc	0.0000477	Pa×s	827.12	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=U355312&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