Sebacic acid, octyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C20H35Cl3O4/c1-2-3-4-5-10-13-16-26-18(24)14-11-8-6-7-9-12-15-19(25)27-17
InchiKey: BCFQVGPTFOCQAV-UHFFFAOYSA-N
Formula: C20H35Cl3O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 445.85

Physical Properties

Property code	Value	Unit	Source
gf	-383.27	kJ/mol	Joback Method
hf	-1001.70	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	90.28	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.924		Crippen Method
mcvol	344.260	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	2821.00		NIST Webbook
rinpol	2821.00		NIST Webbook
tb	918.64	K	Joback Method
tc	1125.13	K	Joback Method
tf	551.66	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.01	J/mol×K	918.64	Joback Method
cpg	1123.99	J/mol×K	1090.71	Joback Method
cpg	1112.83	J/mol×K	1056.30	Joback Method
cpg	1100.70	J/mol×K	1021.88	Joback Method
cpg	1087.56	J/mol×K	987.47	Joback Method
cpg	1073.34	J/mol×K	953.05	Joback Method
cpg	1134.22	J/mol×K	1125.13	Joback Method
dvisc	0.0000249	Pa×s	918.64	Joback Method

dvisc	0.0000331	Pa×s	857.48	Joback Method
dvisc	0.0000461	Pa×s	796.31	Joback Method
dvisc	0.0000677	Pa×s	735.15	Joback Method
dvisc	0.0001068	Pa×s	673.99	Joback Method
dvisc	0.0001842	Pa×s	612.82	Joback Method
dvisc	0.0003588	Pa×s	551.66	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=U355316&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