

Sebacic acid, decyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C22H39Cl3O4/c1-2-3-4-5-6-9-12-15-18-28-20(26)16-13-10-7-8-11-14-17-21(27)
InchiKey: WJXQQWJYBKBJLI-UHFFFAOYSA-N
Formula: C22H39Cl3O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 473.90

Physical Properties

Property code	Value	Unit	Source
gf	-366.43	kJ/mol	Joback Method
hf	-1042.98	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	94.74	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.704		Crippen Method
mcvol	372.440	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpol	3026.00		NIST Webbook
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tb	964.40	K	Joback Method
tc	1181.25	K	Joback Method
tf	574.20	K	Joback Method
vc	1.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.72	J/molxK	964.40	Joback Method
cpg	1248.57	J/molxK	1145.11	Joback Method
cpg	1237.07	J/molxK	1108.97	Joback Method
cpg	1224.49	J/molxK	1072.83	Joback Method
cpg	1210.78	J/molxK	1036.68	Joback Method
cpg	1195.88	J/molxK	1000.54	Joback Method
cpg	1259.08	J/molxK	1181.25	Joback Method
dvisc	0.0000179	Paxs	964.40	Joback Method

dvisc	0.0000239	Paxs	899.37	Joback Method
dvisc	0.0000334	Paxs	834.33	Joback Method
dvisc	0.0000495	Paxs	769.30	Joback Method
dvisc	0.0000787	Paxs	704.27	Joback Method
dvisc	0.0001377	Paxs	639.23	Joback Method
dvisc	0.0002736	Paxs	574.20	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=U355318&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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