

Sebacic acid, nonyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C21H37Cl3O4/c1-2-3-4-5-8-11-14-17-27-19(25)15-12-9-6-7-10-13-16-20(26)21
InchiKey:	BHVDTTHQSZEMBA-UHFFFAOYSA-N
Formula:	C21H37Cl3O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	459.88

Physical Properties

Property code	Value	Unit	Source
gf	-374.85	kJ/mol	Joback Method
hf	-1022.34	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.314		Crippen Method
mvol	358.350	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	2922.00		NIST Webbook
rinpol	2922.00		NIST Webbook
tb	941.52	K	Joback Method
tc	1152.69	K	Joback Method
tf	562.93	K	Joback Method
vc	1.395	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.57	J/molxK	941.52	Joback Method
cpg	1185.95	J/molxK	1117.49	Joback Method
cpg	1174.62	J/molxK	1082.30	Joback Method
cpg	1162.27	J/molxK	1047.10	Joback Method
cpg	1148.85	J/molxK	1011.91	Joback Method
cpg	1134.30	J/molxK	976.71	Joback Method
cpg	1196.32	J/molxK	1152.69	Joback Method
dvisc	0.0000211	Paxs	941.52	Joback Method

dvisc	0.0000281	Paxs	878.42	Joback Method
dvisc	0.0000393	Paxs	815.32	Joback Method
dvisc	0.0000579	Paxs	752.23	Joback Method
dvisc	0.0000917	Paxs	689.13	Joback Method
dvisc	0.0001594	Paxs	626.03	Joback Method
dvisc	0.0003137	Paxs	562.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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