Adipic acid, nonyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C17H29Cl3O4/c1-2-3-4-5-6-7-10-13-23-15(21)11-8-9-12-16(22)24-14-17(18,19
InchiKey: XEYOSPYENLASBY-UHFFFAOYSA-N
Formula: C17H29Cl3O4
SMILES: CCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 403.77

Physical Properties

Property code	Value	Unit	Source
gf	-408.53	kJ/mol	Joback Method
hf	-939.78	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	83.61	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.754		Crippen Method
mcvol	301.990	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	850.00	K	Joback Method
tc	1047.84	K	Joback Method
tf	517.85	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.37	J/mol×K	850.00	Joback Method
cpg	894.63	J/mol×K	882.97	Joback Method
cpg	907.93	J/mol×K	915.95	Joback Method
cpg	920.29	J/mol×K	948.92	Joback Method
cpg	931.76	J/mol×K	981.89	Joback Method
cpg	942.37	J/mol×K	1014.86	Joback Method
cpg	952.15	J/mol×K	1047.84	Joback Method
dvisc	0.0005291	Pa×s	517.85	Joback Method

dvisc	0.0002806	Pa×s	573.21	Joback Method
dvisc	0.0001663	Pa×s	628.57	Joback Method
dvisc	0.0001073	Pa×s	683.92	Joback Method
dvisc	0.0000740	Pa×s	739.28	Joback Method
dvisc	0.0000537	Pa×s	794.64	Joback Method
dvisc	0.0000406	Pa×s	850.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353481&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

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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