Diethylmalonic acid, 2,2-dichloroethyl nonyl ester

Inchi: InChI=1S/C18H32Cl2O4/c1-4-7-8-9-10-11-12-13-23-16(21)18(5-2,6-3)17(22)24-14-15(19

InchiKey: GDGLHRYDEAUTSE-UHFFFAOYSA-N

Formula: C18H32Cl2O4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 383.35

Physical Properties

Property code	Value	Unit	Source
gf	-390.62	kJ/mol	Joback Method
hf	-949.96	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	81.06	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.433		Crippen Method
mcvol	303.840	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	2205.00		NIST Webbook
tb	835.01	K	Joback Method
tc	1030.08	K	Joback Method
tf	484.20	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.14	J/mol×K	835.01	Joback Method
cpg	980.70	J/mol×K	997.57	Joback Method
cpg	968.90	J/mol×K	965.06	Joback Method
cpg	956.17	J/mol×K	932.54	Joback Method
cpg	942.49	J/mol×K	900.03	Joback Method
cpg	927.83	J/mol×K	867.52	Joback Method
cpg	991.62	J/mol×K	1030.08	Joback Method
dvisc	0.0000380	Pa×s	835.01	Joback Method
dvisc	0.0000515	Pa×s	776.54	Joback Method

dvisc	0.0000732	Pa×s	718.07	Joback Method
dvisc	0.0001109	Pa×s	659.61	Joback Method
dvisc	0.0001821	Pa×s	601.14	Joback Method
dvisc	0.0003328	Pa×s	542.67	Joback Method
dvisc	0.0007032	Pa×s	484.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370784&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