

Diethylmalonic acid, 2,2-dichloroethyl hexyl ester

Inchi: InChI=1S/C15H26Cl2O4/c1-4-7-8-9-10-20-13(18)15(5-2,6-3)14(19)21-11-12(16)17/h12H
InchiKey: DTOYZLQISNGCMX-UHFFFAOYSA-N
Formula: C15H26Cl2O4
SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 341.27

Physical Properties

Property code	Value	Unit	Source
gf	-415.88	kJ/mol	Joback Method
hf	-888.04	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	74.38	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.263		Crippen Method
mcvol	261.570	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	1899.00		NIST Webbook
tb	766.37	K	Joback Method
tc	959.76	K	Joback Method
tf	450.39	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.60	J/molxK	766.37	Joback Method
cpg	754.34	J/molxK	798.60	Joback Method
cpg	768.17	J/molxK	830.83	Joback Method
cpg	781.10	J/molxK	863.07	Joback Method
cpg	793.18	J/molxK	895.30	Joback Method
cpg	804.42	J/molxK	927.53	Joback Method
cpg	814.85	J/molxK	959.76	Joback Method
dvisc	0.0010231	Paxs	450.39	Joback Method
dvisc	0.0005000	Paxs	503.05	Joback Method

dvisc	0.0002799	Paxs	555.72	Joback Method
dvisc	0.0001732	Paxs	608.38	Joback Method
dvisc	0.0001157	Paxs	661.04	Joback Method
dvisc	0.0000820	Paxs	713.71	Joback Method
dvisc	0.0000610	Paxs	766.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370781&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
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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