Diglycolic acid, 2,4-dichloronaphth-1-yl ethyl ester

Inchi: InChI=1S/C16H14Cl2O5/c1-2-22-14(19)8-21-9-15(20)23-16-11-6-4-3-5-10(11)12(17)7-13

InchiKey: RNRCTXWRRNCISG-UHFFFAOYSA-N

Formula: C16H14Cl2O5

SMILES: CCOC(=O)COCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 357.19

Physical Properties

Property code	Value	Unit	Source
gf	-322.69	kJ/mol	Joback Method
hf	-633.68	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.632		Crippen Method
mcvol	238.310	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	3178.00		NIST Webbook
rinpol	3178.00		NIST Webbook
tb	875.94	K	Joback Method
tc	1103.53	K	Joback Method
tf	593.15	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.87	J/mol×K	875.94	Joback Method
cpg	688.28	J/mol×K	1065.60	Joback Method
cpg	681.79	J/mol×K	1027.67	Joback Method
cpg	674.31	J/mol×K	989.73	Joback Method
cpg	665.85	J/mol×K	951.80	Joback Method
cpg	656.37	J/mol×K	913.87	Joback Method
cpg	693.81	J/mol×K	1103.53	Joback Method
dvisc	0.0001109	Pa×s	875.94	Joback Method

dvisc	0.0001313	Pa×s	828.81	Joback Method
dvisc	0.0001586	Pa×s	781.68	Joback Method
dvisc	0.0001963	Pa×s	734.55	Joback Method
dvisc	0.0002503	Pa×s	687.41	Joback Method
dvisc	0.0003307	Pa×s	640.28	Joback Method
dvisc	0.0004566	Pa×s	593.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382628&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