

Diglycolic acid, propyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O5/c1-2-3-20-11(17)6-19-7-12(18)21-13-9(15)4-8(14)5-10(13)16/h
InchiKey:	IRYCTTVNVHSBRD-UHFFFAOYSA-N
Formula:	C13H13Cl3O5
SMILES:	CCCOC(=O)COCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	355.60

Physical Properties

Property code	Value	Unit	Source
gf	-466.53	kJ/mol	Joback Method
hf	-778.57	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.522		Crippen Method
mvol	227.740	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rmpol	2742.00		NIST Webbook
rmpol	2742.00		NIST Webbook
tb	825.75	K	Joback Method
tc	1044.21	K	Joback Method
tf	556.56	K	Joback Method
vc	0.869	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.66	J/molxK	825.75	Joback Method
cpg	621.97	J/molxK	1007.80	Joback Method
cpg	615.70	J/molxK	971.39	Joback Method
cpg	608.42	J/molxK	934.98	Joback Method
cpg	600.14	J/molxK	898.57	Joback Method
cpg	590.88	J/molxK	862.16	Joback Method
cpg	627.21	J/molxK	1044.21	Joback Method
dvisc	0.0000731	Paxs	825.75	Joback Method

dvisc	0.0000887	Paxs	780.88	Joback Method
dvisc	0.0001102	Paxs	736.02	Joback Method
dvisc	0.0001409	Paxs	691.15	Joback Method
dvisc	0.0001865	Paxs	646.29	Joback Method
dvisc	0.0002572	Paxs	601.43	Joback Method
dvisc	0.0003737	Paxs	556.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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