

Diglycolic acid, 2,4-dichlorophenyl pentyl ester

Inchi:	InChI=1S/C15H18Cl2O5/c1-2-3-4-7-21-14(18)9-20-10-15(19)22-13-6-5-11(16)8-12(13)17
InchiKey:	SBBPWBBOSRNDOP-UHFFFAOYSA-N
Formula:	C15H18Cl2O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	349.21

Physical Properties

Property code	Value	Unit	Source
gf	-428.13	kJ/mol	Joback Method
hf	-792.64	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.649		Crippen Method
mcvol	243.680	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpola	3100.00		NIST Webbook
rinpola	3100.00		NIST Webbook
tb	829.10	K	Joback Method
tc	1040.04	K	Joback Method
tf	536.66	K	Joback Method
vc	0.931	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.63	J/molxK	829.10	Joback Method
cpg	681.71	J/molxK	864.26	Joback Method
cpg	692.77	J/molxK	899.41	Joback Method
cpg	702.79	J/molxK	934.57	Joback Method
cpg	711.77	J/molxK	969.73	Joback Method
cpg	719.71	J/molxK	1004.89	Joback Method
cpg	726.60	J/molxK	1040.04	Joback Method
dvisc	0.0004117	Paxs	536.66	Joback Method

dvisc	0.0002643	Paxs	585.40	Joback Method
dvisc	0.0001817	Paxs	634.14	Joback Method
dvisc	0.0001318	Paxs	682.88	Joback Method
dvisc	0.0000997	Paxs	731.62	Joback Method
dvisc	0.0000782	Paxs	780.36	Joback Method
dvisc	0.0000630	Paxs	829.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381988&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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