

Diglycolic acid, 2,6-dichlorophenyl nonyl ester

Inchi:	InChI=1S/C19H26Cl2O5/c1-2-3-4-5-6-7-8-12-25-17(22)13-24-14-18(23)26-19-15(20)10-9
InchiKey:	UDFTVFWARDPCOY-UHFFFAOYSA-N
Formula:	C19H26Cl2O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	405.31

Physical Properties

Property code	Value	Unit	Source
gf	-394.45	kJ/mol	Joback Method
hf	-875.20	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	90.98	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.209		Crippen Method
mvol	300.040	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	3358.00		NIST Webbook
rinpol	3358.00		NIST Webbook
tb	920.62	K	Joback Method
tc	1132.87	K	Joback Method
tf	581.74	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.85	J/molxK	920.62	Joback Method
cpg	910.74	J/molxK	955.99	Joback Method
cpg	922.38	J/molxK	991.37	Joback Method
cpg	932.77	J/molxK	1026.74	Joback Method
cpg	941.91	J/molxK	1062.12	Joback Method
cpg	949.82	J/molxK	1097.49	Joback Method
cpg	956.49	J/molxK	1132.87	Joback Method
dvisc	0.0002727	Paxs	581.74	Joback Method

dvisc	0.0001668	Paxs	638.22	Joback Method
dvisc	0.0001105	Paxs	694.70	Joback Method
dvisc	0.0000779	Paxs	751.18	Joback Method
dvisc	0.0000577	Paxs	807.66	Joback Method
dvisc	0.0000444	Paxs	864.14	Joback Method
dvisc	0.0000353	Paxs	920.62	Joback Method

Sources

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=U382304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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