

Diglycolic acid, 2,6-dimethoxyphenyl octyl ester

Inchi:	InChI=1S/C20H30O7/c1-4-5-6-7-8-9-13-26-18(21)14-25-15-19(22)27-20-16(23-2)11-10-
InchiKey:	RTOIXSDLQLPZRH-UHFFFAOYSA-N
Formula:	C20H30O7
SMILES:	CCCCCCCCOC(=O)COCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	382.45

Physical Properties

Property code	Value	Unit	Source
gf	-572.17	kJ/mol	Joback Method
hf	-1128.80	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	89.26	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.529		Crippen Method
mcvol	301.390	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinqol	3339.00		NIST Webbook
tb	913.48	K	Joback Method
tc	1120.85	K	Joback Method
tf	577.63	K	Joback Method
vc	1.149	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.04	J/molxK	913.48	Joback Method
cpg	1020.52	J/molxK	1086.29	Joback Method
cpg	1012.29	J/molxK	1051.72	Joback Method
cpg	1002.51	J/molxK	1017.16	Joback Method
cpg	991.19	J/molxK	982.60	Joback Method
cpg	978.36	J/molxK	948.04	Joback Method
cpg	1027.17	J/molxK	1120.85	Joback Method
dvisc	0.0000232	Paxs	913.48	Joback Method
dvisc	0.0000292	Paxs	857.50	Joback Method

dvisc	0.0000380	Paxs	801.53	Joback Method
dvisc	0.0000515	Paxs	745.56	Joback Method
dvisc	0.0000731	Paxs	689.58	Joback Method
dvisc	0.0001106	Paxs	633.61	Joback Method
dvisc	0.0001812	Paxs	577.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381910&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
mvol:	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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