

Diglycolic acid, 2-isopropoxyphenyl pentyl ester

Inchi:	InChI=1S/C18H26O6/c1-4-5-8-11-22-17(19)12-21-13-18(20)24-16-10-7-6-9-15(16)23-14
InchiKey:	SSFKSUPWOHGLB-UHFFFAOYSA-N
Formula:	C18H26O6
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	338.40

Physical Properties

Property code	Value	Unit	Source
gf	-476.82	kJ/mol	Joback Method
hf	-949.11	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	81.34	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.129		Crippen Method
mvol	267.340	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2992.00		NIST Webbook
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tb	839.88	K	Joback Method
tc	1042.54	K	Joback Method
tf	505.34	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.17	J/molxK	839.88	Joback Method
cpg	834.06	J/molxK	873.66	Joback Method
cpg	847.75	J/molxK	907.43	Joback Method
cpg	860.21	J/molxK	941.21	Joback Method
cpg	871.45	J/molxK	974.98	Joback Method
cpg	881.45	J/molxK	1008.76	Joback Method
cpg	890.21	J/molxK	1042.54	Joback Method
dvisc	0.0004011	Paxs	505.34	Joback Method

dvisc	0.0002221	Paxs	561.10	Joback Method
dvisc	0.0001369	Paxs	616.85	Joback Method
dvisc	0.0000914	Paxs	672.61	Joback Method
dvisc	0.0000649	Paxs	728.37	Joback Method
dvisc	0.0000484	Paxs	784.12	Joback Method
dvisc	0.0000375	Paxs	839.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log_p:	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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