Diglycolic acid, isobutyl 2-naphthyl ester

Inchi: InChI=1S/C18H20O5/c1-13(2)10-22-17(19)11-21-12-18(20)23-16-8-7-14-5-3-4-6-15(14)9
InchiKey: QUPRDQJWLDRLSQ-UHFFFAOYSA-N
Formula: C18H20O5
SMILES: CC(C)COC(=O)COCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 316.35

Physical Properties

Property code	Value	Unit	Source
gf	-265.17	kJ/mol	Joback Method
hf	-625.82	kJ/mol	Joback Method
hfus	36.29	kJ/mol	Joback Method
hvap	80.57	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.961		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook
tb	836.44	K	Joback Method
tc	1054.86	K	Joback Method
tf	515.81	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.61	J/mol×K	836.44	Joback Method
cpg	730.34	J/mol×K	872.84	Joback Method
cpg	742.95	J/mol×K	909.25	Joback Method
cpg	754.46	J/mol×K	945.65	Joback Method
cpg	764.92	J/mol×K	982.06	Joback Method
cpg	774.34	J/mol×K	1018.46	Joback Method
cpg	782.77	J/mol×K	1054.86	Joback Method
dvisc	0.0006655	Pa×s	515.81	Joback Method

dvisc	0.0004157	Pa×s	569.25	Joback Method
dvisc	0.0002815	Pa×s	622.69	Joback Method
dvisc	0.0002027	Pa×s	676.12	Joback Method
dvisc	0.0001532	Pa×s	729.56	Joback Method
dvisc	0.0001202	Pa×s	783.00	Joback Method
dvisc	0.0000974	Pa×s	836.44	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=U381787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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