

Diglycolic acid, 2-naphthyl pentyl ester

Inchi:	InChI=1S/C19H22O5/c1-2-3-6-11-23-18(20)13-22-14-19(21)24-17-10-9-15-7-4-5-8-16(15)
InchiKey:	BPJJTPYNMUTFEG-UHFFFAOYSA-N
Formula:	C19H22O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	330.38

Physical Properties

Property code	Value	Unit	Source
gf	-254.31	kJ/mol	Joback Method
hf	-641.18	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.495		Crippen Method
mcvol	256.100	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinsol	3269.00		NIST Webbook
tb	859.76	K	Joback Method
tc	1074.24	K	Joback Method
tf	542.08	K	Joback Method
vc	0.980	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.93	J/molxK	859.76	Joback Method
cpg	786.71	J/molxK	895.51	Joback Method
cpg	799.38	J/molxK	931.25	Joback Method
cpg	810.97	J/molxK	967.00	Joback Method
cpg	821.52	J/molxK	1002.74	Joback Method
cpg	831.05	J/molxK	1038.49	Joback Method
cpg	839.60	J/molxK	1074.24	Joback Method
dvisc	0.0005668	Paxs	542.08	Joback Method
dvisc	0.0003673	Paxs	595.03	Joback Method

dvisc	0.0002555	Paxs	647.97	Joback Method
dvisc	0.0001878	Paxs	700.92	Joback Method
dvisc	0.0001441	Paxs	753.87	Joback Method
dvisc	0.0001145	Paxs	806.81	Joback Method
dvisc	0.0000936	Paxs	859.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381788&Units=SI

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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