

Diglycolic acid, heptyl 2-naphthyl ester

Inchi:	InChI=1S/C21H26O5/c1-2-3-4-5-8-13-25-20(22)15-24-16-21(23)26-19-12-11-17-9-6-7-10
InchiKey:	MFDGDYQBXSGQKY-UHFFFAOYSA-N
Formula:	C21H26O5
SMILES:	CCCCCCCOC(=O)COCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	358.43

Physical Properties

Property code	Value	Unit	Source
gf	-237.47	kJ/mol	Joback Method
hf	-682.46	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.275		Crippen Method
mcvol	284.280	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	3491.00		NIST Webbook
rinpol	3491.00		NIST Webbook
tb	905.52	K	Joback Method
tc	1119.84	K	Joback Method
tf	564.62	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.06	J/molxK	905.52	Joback Method
cpg	903.20	J/molxK	941.24	Joback Method
cpg	916.17	J/molxK	976.96	Joback Method
cpg	928.00	J/molxK	1012.68	Joback Method
cpg	938.74	J/molxK	1048.40	Joback Method
cpg	948.41	J/molxK	1084.12	Joback Method
cpg	957.07	J/molxK	1119.84	Joback Method
dvisc	0.0004745	Paxs	564.62	Joback Method

dvisc	0.0003000	Paxs	621.44	Joback Method
dvisc	0.0002049	Paxs	678.25	Joback Method
dvisc	0.0001484	Paxs	735.07	Joback Method
dvisc	0.0001125	Paxs	791.89	Joback Method
dvisc	0.0000886	Paxs	848.70	Joback Method
dvisc	0.0000719	Paxs	905.52	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=U381791&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

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