Glutaric acid, 1-naphthyl pentyl ester

Inchi: InChI=1S/C20H24O4/c1-2-3-6-15-23-19(21)13-8-14-20(22)24-18-12-7-10-16-9-4-5-11-17
InchiKey: BGGPRMSRSYDTTJ-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: CCCCCOC(=O)CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	-140.89	kJ/mol	Joback Method
hf	-529.60	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.649		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	860.22	K	Joback Method
tc	1074.09	K	Joback Method
tf	531.12	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.86	J/mol×K	860.22	Joback Method
cpg	817.37	J/mol×K	895.87	Joback Method
cpg	830.81	J/mol×K	931.51	Joback Method
cpg	843.24	J/mol×K	967.16	Joback Method
cpg	854.70	J/mol×K	1002.80	Joback Method
cpg	865.25	J/mol×K	1038.45	Joback Method
cpg	874.92	J/mol×K	1074.09	Joback Method
dvisc	0.0007126	Pa×s	531.12	Joback Method
dvisc	0.0004495	Pa×s	585.97	Joback Method

dvisc	0.0003068	Pa×s	640.82	Joback Method
dvisc	0.0002224	Pa×s	695.67	Joback Method
dvisc	0.0001690	Pa×s	750.52	Joback Method
dvisc	0.0001333	Pa×s	805.37	Joback Method
dvisc	0.0001084	Pa×s	860.22	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=U358766&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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