

Glutaric acid, naphth-2-ylmethyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C22H28O4/c1-16(2)13-17(3)26-22(24)10-6-9-21(23)25-15-18-11-12-19-7-4-5-8
InchiKey:	IZDUPFLUQJHEAB-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CC(C)CC(C)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	356.46

Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-581.44	kJ/mol	Joback Method
hfus	41.93	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.031		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinqol	2741.00		NIST Webbook
tb	905.10	K	Joback Method
tc	1122.68	K	Joback Method
tf	523.66	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.99	J/molxK	905.10	Joback Method
cpg	985.43	J/molxK	1086.42	Joback Method
cpg	974.66	J/molxK	1050.15	Joback Method
cpg	962.88	J/molxK	1013.89	Joback Method
cpg	950.05	J/molxK	977.63	Joback Method
cpg	936.11	J/molxK	941.36	Joback Method
cpg	995.27	J/molxK	1122.68	Joback Method
dvisc	0.0000696	Paxs	905.10	Joback Method
dvisc	0.0000885	Paxs	841.53	Joback Method

dvisc	0.0001170	Paxs	777.95	Joback Method
dvisc	0.0001626	Paxs	714.38	Joback Method
dvisc	0.0002411	Paxs	650.81	Joback Method
dvisc	0.0003892	Paxs	587.23	Joback Method
dvisc	0.0007057	Paxs	523.66	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=U392506&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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