

Glutaric acid, naphth-2-ylmethyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C24H32O4/c1-18(15-24(2,3)4)16-27-22(25)10-7-11-23(26)28-17-19-12-13-20-
InchiKey:	WYKCMDUXULXVRU-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	CC(COC(=O)CCCC(=O)OCc1ccc2ccccc2c1)CC(C)(C)C
Mol. weight [g/mol]:	384.51

Physical Properties

Property code	Value	Unit	Source
gf	-106.81	kJ/mol	Joback Method
hf	-626.19	kJ/mol	Joback Method
hfus	43.22	kJ/mol	Joback Method
hvap	90.22	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.669		Crippen Method
mcvol	320.680	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinqol	2952.00		NIST Webbook
tb	948.07	K	Joback Method
tc	1169.80	K	Joback Method
tf	563.62	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.63	J/molxK	948.07	Joback Method
cpg	1108.21	J/molxK	1132.85	Joback Method
cpg	1096.58	J/molxK	1095.89	Joback Method
cpg	1084.10	J/molxK	1058.94	Joback Method
cpg	1070.68	J/molxK	1021.98	Joback Method
cpg	1056.22	J/molxK	985.03	Joback Method
cpg	1119.07	J/molxK	1169.80	Joback Method
dvisc	0.0000442	Paxs	948.07	Joback Method
dvisc	0.0000567	Paxs	883.99	Joback Method

dvisc	0.0000758	Paxs	819.92	Joback Method
dvisc	0.0001062	Paxs	755.85	Joback Method
dvisc	0.0001586	Paxs	691.77	Joback Method
dvisc	0.0002569	Paxs	627.69	Joback Method
dvisc	0.0004645	Paxs	563.62	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=U391544&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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