

Glutaric acid, naphth-2-ylmethyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C23H30O4/c1-16(2)23(17(3)4)27-22(25)11-7-10-21(24)26-15-18-12-13-19-8-5
InchiKey: YEJOQBVAQRJAPS-UHFFFAOYSA-N
Formula: C23H30O4
SMILES: CC(C)C(OC(=O)CCCC(=O)OCc1ccc2ccccc2c1)C(C)C
Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-122.95	kJ/mol	Joback Method
hf	-607.36	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	88.52	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.277		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	2844.00		NIST Webbook
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tb	927.54	K	Joback Method
tc	1147.30	K	Joback Method
tf	519.93	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.04	J/molxK	927.54	Joback Method
cpg	1046.18	J/molxK	1110.68	Joback Method
cpg	1035.35	J/molxK	1074.05	Joback Method
cpg	1023.48	J/molxK	1037.42	Joback Method
cpg	1010.52	J/molxK	1000.79	Joback Method
cpg	996.39	J/molxK	964.17	Joback Method
cpg	1056.04	J/molxK	1147.30	Joback Method
dvisc	0.0000553	Paxs	927.54	Joback Method

dvisc	0.0000715	Paxs	859.61	Joback Method
dvisc	0.0000966	Paxs	791.67	Joback Method
dvisc	0.0001380	Paxs	723.74	Joback Method
dvisc	0.0002124	Paxs	655.80	Joback Method
dvisc	0.0003610	Paxs	587.87	Joback Method
dvisc	0.0007049	Paxs	519.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393488&Units=SI
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

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
mccvol:	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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