

Glutaric acid, cyclohexylmethyl (2-naphthyl)methyl ester

Inchi: InChI=1S/C23H28O4/c24-22(26-16-18-7-2-1-3-8-18)11-6-12-23(25)27-17-19-13-14-20-9
InchiKey: SJVLQKRDLIZAIH-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-91.18	kJ/mol	Joback Method
hf	-537.20	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	90.11	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.177		Crippen Method
mcvol	295.730	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	3116.00		NIST Webbook
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tb	948.41	K	Joback Method
tc	1180.53	K	Joback Method
tf	572.31	K	Joback Method
vc	1.119	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.57	J/molxK	948.41	Joback Method
cpg	1036.62	J/molxK	1141.85	Joback Method
cpg	1026.57	J/molxK	1103.16	Joback Method
cpg	1015.32	J/molxK	1064.47	Joback Method
cpg	1002.79	J/molxK	1025.78	Joback Method
cpg	988.90	J/molxK	987.10	Joback Method
cpg	1045.54	J/molxK	1180.53	Joback Method
dvisc	0.0000755	Paxs	948.41	Joback Method

dvisc	0.0000947	Paxs	885.73	Joback Method
dvisc	0.0001227	Paxs	823.04	Joback Method
dvisc	0.0001661	Paxs	760.36	Joback Method
dvisc	0.0002374	Paxs	697.68	Joback Method
dvisc	0.0003640	Paxs	634.99	Joback Method
dvisc	0.0006131	Paxs	572.31	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=U392204&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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