

Glutaric acid, hexa-1,5-dien-3-yl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C22H24O4/c1-3-8-20(4-2)26-22(24)12-7-11-21(23)25-16-17-13-14-18-9-5-6-10
InchiKey:	WQNLADPOGDGRGG-UHFFFAOYSA-N
Formula:	C22H24O4
SMILES:	C=CCC(C=C)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	352.42

Physical Properties

Property code	Value	Unit	Source
gf	49.19	kJ/mol	Joback Method
hf	-325.30	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	85.73	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.727		Crippen Method
mvol	283.900	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2777.00		NIST Webbook
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tb	898.90	K	Joback Method
tc	1118.08	K	Joback Method
tf	535.14	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.89	J/molxK	898.90	Joback Method
cpg	878.04	J/molxK	935.43	Joback Method
cpg	891.14	J/molxK	971.96	Joback Method
cpg	903.27	J/molxK	1008.49	Joback Method
cpg	914.49	J/molxK	1045.02	Joback Method
cpg	924.86	J/molxK	1081.55	Joback Method
cpg	934.47	J/molxK	1118.08	Joback Method
dvisc	0.0006810	Paxs	535.14	Joback Method

dvisc	0.0004067	Paxs	595.77	Joback Method
dvisc	0.0002672	Paxs	656.39	Joback Method
dvisc	0.0001884	Paxs	717.02	Joback Method
dvisc	0.0001403	Paxs	777.65	Joback Method
dvisc	0.0001091	Paxs	838.27	Joback Method
dvisc	0.0000877	Paxs	898.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405291&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
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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