

Glutaric acid, naphth-2-ylmethyl cis-4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C26H34O4/c1-26(2,3)22-13-15-23(16-14-22)30-25(28)10-6-9-24(27)29-18-19-
InchiKey:	UOHDIPOCWYIYOMP-UHFFFAOYSA-N
Formula:	C26H34O4
SMILES:	CC(C)(C)C1CCC(OC(=O)CCCC(=O)OCc2ccc3ccccc3c2)CC1
Mol. weight [g/mol]:	410.55

Physical Properties

Property code	Value	Unit	Source
gf	-70.79	kJ/mol	Joback Method
hf	-628.21	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	95.18	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.201		Crippen Method
mvol	338.000	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	1009.15	K	Joback Method
tc	1246.15	K	Joback Method
tf	604.30	K	Joback Method
vc	1.274	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.46	J/molxK	1009.15	Joback Method
cpg	1225.90	J/molxK	1206.65	Joback Method
cpg	1215.28	J/molxK	1167.15	Joback Method
cpg	1203.54	J/molxK	1127.65	Joback Method
cpg	1190.57	J/molxK	1088.15	Joback Method
cpg	1176.24	J/molxK	1048.65	Joback Method
cpg	1235.50	J/molxK	1246.15	Joback Method
dvisc	0.0000500	Paxs	1009.15	Joback Method

dvisc	0.0000632	Paxs	941.67	Joback Method
dvisc	0.0000828	Paxs	874.20	Joback Method
dvisc	0.0001135	Paxs	806.72	Joback Method
dvisc	0.0001648	Paxs	739.25	Joback Method
dvisc	0.0002579	Paxs	671.77	Joback Method
dvisc	0.0004462	Paxs	604.30	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=U393394&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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