Glutaric acid, naphth-2-ylmethyl trans-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: UOHDIPOCWIYOMP-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
mcvol	338.000	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	3359.00		NIST Webbook
rinpol	3359.00		NIST Webbook
tb	1009.15	K	Joback Method
tc	1246.15	K	Joback Method
tf	604.30	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.46	J/mol×K	1009.15	Joback Method
cpg	1176.24	J/mol×K	1048.65	Joback Method
cpg	1190.57	J/mol×K	1088.15	Joback Method
cpg	1203.54	J/mol×K	1127.65	Joback Method
cpg	1215.28	J/mol×K	1167.15	Joback Method
cpg	1225.90	J/mol×K	1206.65	Joback Method
cpg	1235.50	J/mol×K	1246.15	Joback Method
dvisc	0.0004462	Pa×s	604.30	Joback Method

dvisc	0.0002579	Pa×s	671.77	Joback Method
dvisc	0.0001648	Pa×s	739.25	Joback Method
dvisc	0.0001135	Pa×s	806.72	Joback Method
dvisc	0.0000828	Pa×s	874.20	Joback Method
dvisc	0.0000632	Pa×s	941.67	Joback Method
dvisc	0.0000500	Pa×s	1009.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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