

Glutaric acid, tridec-2-yn-1-yl trans-4-tert-butylcyclohexyl ester

Inchi:	InChI=1S/C28H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-23-31-26(29)17-16-18-27(30)32-2
InchiKey:	PZUGPHAXGQXGAD-UHFFFAOYSA-N
Formula:	C28H48O4
SMILES:	CCCCCCCCC#CCOC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]:	448.68

Physical Properties

Property code	Value	Unit	Source
gf	-60.58	kJ/mol	Joback Method
hf	-813.32	kJ/mol	Joback Method
hfus	62.46	kJ/mol	Joback Method
hvap	97.21	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.382		Crippen Method
mcvol	400.800	ml/mol	McGowan Method
pc	833.86	kPa	Joback Method
rinpol	3229.00		NIST Webbook
rinpol	3229.00		NIST Webbook
tb	1013.27	K	Joback Method
tc	1240.55	K	Joback Method
tf	661.30	K	Joback Method
vc	1.534	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.07	J/molxK	1013.27	Joback Method
cpg	1437.02	J/molxK	1051.15	Joback Method
cpg	1454.17	J/molxK	1089.03	Joback Method
cpg	1469.57	J/molxK	1126.91	Joback Method
cpg	1483.31	J/molxK	1164.79	Joback Method
cpg	1495.47	J/molxK	1202.67	Joback Method
cpg	1506.11	J/molxK	1240.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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