

Glutaric acid, 2-(cyclohexyl)ethyl tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C26H44O4/c1-2-3-4-5-6-7-8-9-10-11-15-22-29-25(27)19-16-20-26(28)30-23-2
InchiKey:	CRHYQLJWNQOKRK-UHFFFAOYSA-N
Formula:	C26H44O4
SMILES:	CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCC1CCCCC1
Mol. weight [g/mol]:	420.63

Physical Properties

Property code	Value	Unit	Source
gf	-72.55	kJ/mol	Joback Method
hf	-742.95	kJ/mol	Joback Method
hfus	63.63	kJ/mol	Joback Method
hvap	94.36	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.748		Crippen Method
mvol	372.620	ml/mol	McGowan Method
pc	942.68	kPa	Joback Method
rinpol	3041.00		NIST Webbook
rinpol	3041.00		NIST Webbook
tb	975.41	K	Joback Method
tc	1194.30	K	Joback Method
tf	640.58	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.98	J/mol×K	975.41	Joback Method
cpg	1305.55	J/mol×K	1011.89	Joback Method
cpg	1322.43	J/mol×K	1048.37	Joback Method
cpg	1337.66	J/mol×K	1084.85	Joback Method
cpg	1351.28	J/mol×K	1121.33	Joback Method
cpg	1363.35	J/mol×K	1157.82	Joback Method
cpg	1373.91	J/mol×K	1194.30	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=U405424&Units=SI

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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