

Glutaric acid, tridec-2-yn-1-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C25H44O5/c1-4-5-6-7-8-9-10-11-12-13-14-20-29-24(26)16-15-17-25(27)30-22
InchiKey: MDPWLCBWQPESDE-UHFFFAOYSA-N
Formula: C25H44O5
SMILES: CCCCCCCCCC#CCOC(=O)CCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]: 424.61

Physical Properties

Property code	Value	Unit	Source
gf	-212.86	kJ/mol	Joback Method
hf	-914.13	kJ/mol	Joback Method
hfus	66.87	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.840		Crippen Method
mvol	375.260	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	954.96	K	Joback Method
tc	1170.25	K	Joback Method
tf	629.16	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.04	J/molxK	954.96	Joback Method
cpg	1277.59	J/molxK	990.84	Joback Method
cpg	1294.50	J/molxK	1026.72	Joback Method
cpg	1309.82	J/molxK	1062.61	Joback Method
cpg	1323.55	J/molxK	1098.49	Joback Method
cpg	1335.72	J/molxK	1134.37	Joback Method
cpg	1346.36	J/molxK	1170.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393533&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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