

Glutaric acid, pent-2-en-1-yl tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C23H38O4/c1-3-5-7-8-9-10-11-12-13-14-16-21-27-23(25)19-17-18-22(24)26-2
InchiKey:	OVEVEVSYMSONQZ-GIDUJCDVSA-N
Formula:	C23H38O4
SMILES:	CCC=CCOC(=O)CCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]:	378.55

Physical Properties

Property code	Value	Unit	Source
gf	-42.04	kJ/mol	Joback Method
hf	-618.13	kJ/mol	Joback Method
hfus	64.22	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.743		Crippen Method
mvol	336.910	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	891.38	K	Joback Method
tc	1092.62	K	Joback Method
tf	594.31	K	Joback Method
vc	1.313	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.54	J/molxK	891.38	Joback Method
cpg	1093.40	J/molxK	924.92	Joback Method
cpg	1110.11	J/molxK	958.46	Joback Method
cpg	1125.70	J/molxK	992.00	Joback Method
cpg	1140.21	J/molxK	1025.54	Joback Method
cpg	1153.68	J/molxK	1059.08	Joback Method
cpg	1166.14	J/molxK	1092.62	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=U405267&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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