Glutaric acid, tridec-2-yn-1-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C25H44O4/c1-5-7-8-9-10-11-12-13-14-15-16-21-28-24(26)19-17-20-25(27)29-

InchiKey: MINHKHDCLHKHON-UHFFFAOYSA-N

Formula: C25H44O4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC(CCC)C(C)C

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-110.30	kJ/mol	Joback Method
hf	-787.19	kJ/mol	Joback Method
hfus	62.16	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.602		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	932.10	K	Joback Method
tc	1141.17	K	Joback Method
tf	591.93	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.36	J/mol×K	932.10	Joback Method
cpg	1247.39	J/mol×K	966.95	Joback Method
cpg	1264.96	J/mol×K	1001.79	Joback Method
cpg	1281.13	J/mol×K	1036.64	Joback Method
cpg	1295.93	J/mol×K	1071.48	Joback Method
cpg	1309.38	J/mol×K	1106.33	Joback Method
cpg	1321.53	J/mol×K	1141.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393849&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
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
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