Glutaric acid, tridec-2-yn-1-yl 4-methylpent-2-yl ester

Inchi: InChI=1S/C24H42O4/c1-5-6-7-8-9-10-11-12-13-14-15-19-27-23(25)17-16-18-24(26)28-2
InchiKey: QZLOEMGXWOHBLR-UHFFFAOYSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-118.72	kJ/mol	Joback Method
hf	-766.55	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	88.71	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.212		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	909.22	K	Joback Method
tc	1113.45	K	Joback Method
tf	580.66	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.63	J/mol×K	909.22	Joback Method
cpg	1184.33	J/mol×K	943.26	Joback Method
cpg	1201.67	J/mol×K	977.30	Joback Method
cpg	1217.69	J/mol×K	1011.34	Joback Method
cpg	1232.42	J/mol×K	1045.37	Joback Method
cpg	1245.89	J/mol×K	1079.41	Joback Method
cpg	1258.12	J/mol×K	1113.45	Joback Method

Sources

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=U392505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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