Glutaric acid, tridec-2-yn-1-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C25H44O4/c1-6-7-8-9-10-11-12-13-14-15-16-20-28-23(26)18-17-19-24(27)29-

InchiKey: YQNNWTVICNHAMJ-UHFFFAOYSA-N

Formula: C25H44O4

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

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-112.74	kJ/mol	Joback Method
hf	-792.47	kJ/mol	Joback Method
hfus	58.63	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.458		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	895.34	kPa	Joback Method
rinpol	2727.00		NIST Webbook
tb	931.66	K	Joback Method
tc	1140.63	K	Joback Method
tf	576.93	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1228.76	J/mol×K	931.66	Joback Method
cpg	1247.74	J/mol×K	966.49	Joback Method
cpg	1265.27	J/mol×K	1001.32	Joback Method
cpg	1281.37	J/mol×K	1036.15	Joback Method
cpg	1296.09	J/mol×K	1070.97	Joback Method
cpg	1309.46	J/mol×K	1105.80	Joback Method
cpg	1321.51	J/mol×K	1140.63	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=U393487&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