Glutaric acid, tridec-2-yn-1-yl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C28H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-23-31-27(29)20-17-21-28(30)32-2
InchiKey: OHCYLBXPJGKFIO-UHFFFAOYSA-N
Formula: C28H50O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-85.04	kJ/mol	Joback Method
hf	-849.11	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	7.630		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	1000.74	K	Joback Method
tc	1230.70	K	Joback Method
tf	625.74	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.28	J/mol×K	1000.74	Joback Method
cpg	1439.46	J/mol×K	1039.07	Joback Method
cpg	1457.84	J/mol×K	1077.39	Joback Method
cpg	1474.46	J/mol×K	1115.72	Joback Method
cpg	1489.39	J/mol×K	1154.05	Joback Method
cpg	1502.67	J/mol×K	1192.37	Joback Method
cpg	1514.38	J/mol×K	1230.70	Joback Method

Sources

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=U391494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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