Glutaric acid, di(tridec-2-ynyl) ester

Inchi: InChI=1S/C31H52O4/c1-3-5-7-9-11-13-15-17-19-21-23-28-34-30(32)26-25-27-31(33)35-
InchiKey: WJYYNLNKYUALCD-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	147.90	kJ/mol	Joback Method
hf	-628.17	kJ/mol	Joback Method
hfus	87.86	kJ/mol	Joback Method
hvap	107.22	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	8.312		Crippen Method
mcvol	445.330	ml/mol	McGowan Method
pc	699.13	kPa	Joback Method
rinpol	3620.00		NIST Webbook
rinpol	3620.00		NIST Webbook
tb	1079.26	K	Joback Method
tc	1337.04	K	Joback Method
tf	795.65	K	Joback Method
vc	1.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.42	J/mol×K	1079.26	Joback Method
cpg	1574.47	J/mol×K	1122.22	Joback Method
cpg	1592.36	J/mol×K	1165.19	Joback Method
cpg	1608.18	J/mol×K	1208.15	Joback Method
cpg	1622.01	J/mol×K	1251.11	Joback Method
cpg	1633.95	J/mol×K	1294.07	Joback Method
cpg	1644.08	J/mol×K	1337.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360128&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

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