Glutaric acid, heptadecyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C28H50O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-31-27(29)23-21-
InchiKey: CAGHCEVQZSTNQB-UHFFFAOYSA-N
Formula: C28H50O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-82.60	kJ/mol	Joback Method
hf	-843.83	kJ/mol	Joback Method
hfus	73.45	kJ/mol	Joback Method
hvap	98.00	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	7.916		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	752.26	kPa	Joback Method
rinpol	3178.00		NIST Webbook
tb	1001.18	K	Joback Method
tc	1232.66	K	Joback Method
tf	640.74	K	Joback Method
vc	1.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.98	J/mol×K	1001.18	Joback Method
cpg	1439.36	J/mol×K	1039.76	Joback Method
cpg	1457.92	J/mol×K	1078.34	Joback Method
cpg	1474.71	J/mol×K	1116.92	Joback Method
cpg	1489.80	J/mol×K	1155.50	Joback Method
cpg	1503.25	J/mol×K	1194.08	Joback Method
cpg	1515.12	J/mol×K	1232.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359868&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