Glutaric acid, but-3-yn-2-yl heptyl ester

Inchi: InChI=1S/C16H26O4/c1-4-6-7-8-9-13-19-15(17)11-10-12-16(18)20-14(3)5-2/h2,14H,4,6-
InchiKey: BIKJQEDHGVUSMT-UHFFFAOYSA-N
Formula: C16H26O4
SMILES: C#CC(C)OC(=O)CCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-163.37	kJ/mol	Joback Method
hf	-576.55	kJ/mol	Joback Method
hfus	42.22	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.235		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	707.74	K	Joback Method
tc	892.21	K	Joback Method
tf	446.37	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.18	J/mol×K	707.74	Joback Method
cpg	700.00	J/mol×K	738.48	Joback Method
cpg	715.00	J/mol×K	769.23	Joback Method
cpg	729.19	J/mol×K	799.97	Joback Method
cpg	742.58	J/mol×K	830.72	Joback Method
cpg	755.20	J/mol×K	861.46	Joback Method
cpg	767.05	J/mol×K	892.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359878&Units=SI

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