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

Inchi: InChI=1S/C15H24O4/c1-4-7-12-18-14(16)10-8-11-15(17)19-13(6-3)9-5-2/h13H,4,6-8,10-
InchiKey: UGMUENMAXVCGJG-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCC
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-192.06	kJ/mol	Joback Method
hf	-575.51	kJ/mol	Joback Method
hfus	39.78	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.845		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1864.00		NIST Webbook
tb	703.74	K	Joback Method
tc	896.30	K	Joback Method
tf	494.23	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.25	J/mol×K	703.74	Joback Method
cpg	649.03	J/mol×K	735.83	Joback Method
cpg	663.98	J/mol×K	767.93	Joback Method
cpg	678.10	J/mol×K	800.02	Joback Method
cpg	691.40	J/mol×K	832.12	Joback Method
cpg	703.87	J/mol×K	864.21	Joback Method
cpg	715.53	J/mol×K	896.30	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=U359855&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