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

Inchi: InChI=1S/C15H24O4/c1-5-8-13(6-2)19-15(17)10-7-9-14(16)18-11-12(3)4/h12-13H,6-7,9-
InchiKey: CRTYWRCYZWYOFK-UHFFFAOYSA-N
Formula: C15H24O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-194.50	kJ/mol	Joback Method
hf	-580.79	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.701		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1822.00		NIST Webbook
tb	703.30	K	Joback Method
tc	898.78	K	Joback Method
tf	479.23	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.75	J/mol×K	703.30	Joback Method
cpg	649.79	J/mol×K	735.88	Joback Method
cpg	664.97	J/mol×K	768.46	Joback Method
cpg	679.28	J/mol×K	801.04	Joback Method
cpg	692.74	J/mol×K	833.62	Joback Method
cpg	705.34	J/mol×K	866.20	Joback Method
cpg	717.08	J/mol×K	898.78	Joback Method

Sources

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=U359854&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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