Glutaric acid, hex-4-yn-3-yl 3-methylbut-2-yl ester

Inchi: InChI=1S/C16H26O4/c1-6-9-14(7-2)20-16(18)11-8-10-15(17)19-13(5)12(3)4/h12-14H,7-8

InchiKey: LDTPQGDJTGVNBE-UHFFFAOYSA-N

Formula: C16H26O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-188.52	kJ/mol	Joback Method
hf	-606.71	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.089		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	725.74	K	Joback Method
tc	922.55	K	Joback Method
tf	475.50	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.57	J/mol×K	725.74	Joback Method
cpg	706.24	J/mol×K	758.54	Joback Method
cpg	721.97	J/mol×K	791.34	Joback Method
cpg	736.76	J/mol×K	824.14	Joback Method
cpg	750.61	J/mol×K	856.95	Joback Method
cpg	763.55	J/mol×K	889.75	Joback Method
cpg	775.56	J/mol×K	922.55	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=U393568&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