Glutaric acid, hex-4-yn-3-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C18H30O5/c1-5-8-16(6-2)23-18(20)10-7-9-17(19)22-14-12-15(3)11-13-21-4/h1

InchiKey: XMXVJZOWFJIWID-UHFFFAOYSA-N

Formula: C18H30O5

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

Mol. weight [g/mol]: 326.43

Physical Properties

Property code	Value	Unit	Source
gf	-274.24	kJ/mol	Joback Method
hf	-774.93	kJ/mol	Joback Method
hfus	45.21	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.108		Crippen Method
mcvol	276.630	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	794.36	K	Joback Method
tc	987.61	K	Joback Method
tf	535.27	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.87	J/mol×K	794.36	Joback Method
cpg	849.56	J/mol×K	826.57	Joback Method
cpg	865.20	J/mol×K	858.78	Joback Method
cpg	879.80	J/mol×K	890.98	Joback Method
cpg	893.35	J/mol×K	923.19	Joback Method
cpg	905.86	J/mol×K	955.40	Joback Method
cpg	917.32	J/mol×K	987.61	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=U393522&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