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

Inchi: InChI=1S/C19H32O4/c1-5-9-10-13-17(8-4)23-19(21)15-11-14-18(20)22-16(7-3)12-6-2/h1
InchiKey: YDIHHEUUDWVLMD-UHFFFAOYSA-N
Formula: C19H32O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OC(CC)CCCCC
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-160.82	kJ/mol	Joback Method
hf	-663.35	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.404		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	794.82	K	Joback Method
tc	987.61	K	Joback Method
tf	524.31	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.45	J/mol×K	794.82	Joback Method
cpg	878.77	J/mol×K	826.95	Joback Method
cpg	895.06	J/mol×K	859.08	Joback Method
cpg	910.32	J/mol×K	891.21	Joback Method
cpg	924.57	J/mol×K	923.34	Joback Method
cpg	937.82	J/mol×K	955.48	Joback Method
cpg	950.08	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=U391560&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

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