

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H30O4/c1-4-7-8-9-10-15-21-17(19)13-11-14-18(20)22-16(6-3)12-5-2/h16H

WGVPFVUSRSAQBQ-UHFFFAOYSA-N

C18H30O4

CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCC

310.43

Physical Properties

Property code	Value	Unit	Source
gf	-166.80	kJ/mol	Joback Method
hf	-637.43	kJ/mol	Joback Method
hfus	47.55	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.015		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	772.38	K	Joback Method
tc	962.93	K	Joback Method
tf	528.04	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.48	J/mol×K	772.38	Joback Method
cpg	819.34	J/mol×K	804.14	Joback Method
cpg	835.23	J/mol×K	835.90	Joback Method
cpg	850.17	J/mol×K	867.65	Joback Method
cpg	864.17	J/mol×K	899.41	Joback Method
cpg	877.24	J/mol×K	931.17	Joback Method
cpg	889.39	J/mol×K	962.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359858&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
hvac:	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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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