

Glutaric acid, isobutyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C18H30O4/c1-6-7-9-16(12-14(2)3)22-18(20)11-8-10-17(19)21-13-15(4)5/h14-1
InchiKey:	ZFZJTOQAFMZTTM-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-171.68	kJ/mol	Joback Method
hf	-647.99	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.727		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinsol	3307.00		NIST Webbook
tb	771.50	K	Joback Method
tc	966.35	K	Joback Method
tf	498.04	K	Joback Method
vc	1.036	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.50	J/mol×K	771.50	Joback Method
cpg	820.75	J/mol×K	803.98	Joback Method
cpg	836.98	J/mol×K	836.45	Joback Method
cpg	852.19	J/mol×K	868.93	Joback Method
cpg	866.40	J/mol×K	901.40	Joback Method
cpg	879.61	J/mol×K	933.88	Joback Method
cpg	891.84	J/mol×K	966.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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