

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H30O4/c1-5-7-10-16(14-15(3)4)22-18(20)12-9-11-17(19)21-13-8-6-2/h15-17,20-21,23-24H,25H2

WQAXKYAUGZIMLJ-UHFFFAOYSA-N

C18H30O4

CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCC

310.43

Physical Properties

Property code	Value	Unit	Source
gf	-169.24	kJ/mol	Joback Method
hf	-642.71	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.871		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	3331.00		NIST Webbook
tb	771.94	K	Joback Method
tc	964.57	K	Joback Method
tf	513.04	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.99	J/mol×K	771.94	Joback Method
cpg	820.04	J/mol×K	804.05	Joback Method
cpg	836.09	J/mol×K	836.15	Joback Method
cpg	851.17	J/mol×K	868.26	Joback Method
cpg	865.27	J/mol×K	900.36	Joback Method
cpg	878.41	J/mol×K	932.47	Joback Method
cpg	890.60	J/mol×K	964.57	Joback Method

Sources

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=U359600&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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