

Glutaric acid, but-3-yn-2-yl hexyl ester

Inchi:	InChI=1S/C15H24O4/c1-4-6-7-8-12-18-14(16)10-9-11-15(17)19-13(3)5-2/h2,13H,4,6-12H
InchiKey:	AQUIQNLTUQCXNA-UHFFFAOYSA-N
Formula:	C15H24O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)OCCCCC</chem>
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	-171.79	kJ/mol	Joback Method
hf	-555.91	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.845		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpola	1817.00		NIST Webbook
tb	684.86	K	Joback Method
tc	870.12	K	Joback Method
tf	435.10	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.42	J/molxK	684.86	Joback Method
cpg	644.80	J/molxK	715.74	Joback Method
cpg	659.40	J/molxK	746.61	Joback Method
cpg	673.23	J/molxK	777.49	Joback Method
cpg	686.30	J/molxK	808.37	Joback Method
cpg	698.62	J/molxK	839.25	Joback Method
cpg	710.21	J/molxK	870.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359877&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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