

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

Inchi:	InChI=1S/C17H28O4/c1-4-6-7-8-9-10-14-20-16(18)12-11-13-17(19)21-15(3)5-2/h2,15H,4
InchiKey:	XWSYLQSGJUMZAI-UHFFFAOYSA-N
Formula:	C17H28O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)OCCCCCCCC</chem>
Mol. weight [g/mol]:	296.40

Physical Properties

Property code	Value	Unit	Source
gf	-154.95	kJ/mol	Joback Method
hf	-597.19	kJ/mol	Joback Method
hfus	44.81	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.625		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpola	2012.00		NIST Webbook
tb	730.62	K	Joback Method
tc	914.77	K	Joback Method
tf	457.64	K	Joback Method
vc	0.992	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.13	J/molxK	730.62	Joback Method
cpg	756.35	J/molxK	761.31	Joback Method
cpg	771.70	J/molxK	792.00	Joback Method
cpg	786.22	J/molxK	822.70	Joback Method
cpg	799.90	J/molxK	853.39	Joback Method
cpg	812.77	J/molxK	884.08	Joback Method
cpg	824.84	J/molxK	914.77	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=U359879&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
mccol:	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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