

Glutaric acid, but-3-yn-2-yl 4-chloro-2-methoxyphenyl ester

Inchi:	InChI=1S/C16H17ClO5/c1-4-11(2)21-15(18)6-5-7-16(19)22-13-9-8-12(17)10-14(13)20-3
InchiKey:	AKEUFKOLKNHLQY-UHFFFAOYSA-N
Formula:	C16H17ClO5
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC</chem>
Mol. weight [g/mol]:	324.76

Physical Properties

Property code	Value	Unit	Source
gf	-187.15	kJ/mol	Joback Method
hf	-510.92	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	2.989		Crippen Method
mvol	236.930	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	804.23	K	Joback Method
tc	1021.65	K	Joback Method
tf	549.98	K	Joback Method
vc	0.894	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.33	J/mol×K	804.23	Joback Method
cpg	661.07	J/mol×K	840.47	Joback Method
cpg	672.78	J/mol×K	876.70	Joback Method
cpg	683.45	J/mol×K	912.94	Joback Method
cpg	693.08	J/mol×K	949.18	Joback Method
cpg	701.68	J/mol×K	985.41	Joback Method
cpg	709.23	J/mol×K	1021.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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