

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

Inchi:	InChI=1S/C14H22O4/c1-6-11(4)17-13(15)8-7-9-14(16)18-12(5)10(2)3/h1,10-12H,7-9H2,
InchiKey:	HLHYRIJFXWQJPJ-UHFFFAOYSA-N
Formula:	C14H22O4
SMILES:	C#CC(C)OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	-185.09	kJ/mol	Joback Method
hf	-545.83	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.309		Crippen Method
mvol	214.400	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
tb	661.10	K	Joback Method
tc	853.68	K	Joback Method
tf	393.83	K	Joback Method
vc	0.811	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.87	J/mol×K	661.10	Joback Method
cpg	592.31	J/mol×K	693.20	Joback Method
cpg	606.96	J/mol×K	725.29	Joback Method
cpg	620.80	J/mol×K	757.39	Joback Method
cpg	633.86	J/mol×K	789.49	Joback Method
cpg	646.13	J/mol×K	821.58	Joback Method
cpg	657.64	J/mol×K	853.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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