

Glutaric acid, but-3-yn-2-yl 4-nitrophenyl ester

Inchi: InChI=1S/C15H15NO6/c1-3-11(2)21-14(17)5-4-6-15(18)22-13-9-7-12(8-10-13)16(19)20/
InchiKey: PUNSWYCOQZKNJW-UHFFFAOYSA-N
Formula: C15H15NO6
SMILES: C#CC(C)OC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 305.28

Physical Properties

Property code	Value	Unit	Source
gf	-33.46	kJ/mol	Joback Method
hf	-341.61	kJ/mol	Joback Method
hfus	44.64	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	2.235		Crippen Method
mvol	222.150	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	868.36	K	Joback Method
tc	1104.97	K	Joback Method
tf	617.65	K	Joback Method
vc	0.854	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.80	J/molxK	868.36	Joback Method
cpg	653.97	J/molxK	907.80	Joback Method
cpg	664.02	J/molxK	947.23	Joback Method
cpg	672.97	J/molxK	986.67	Joback Method
cpg	680.85	J/molxK	1026.10	Joback Method
cpg	687.69	J/molxK	1065.54	Joback Method
cpg	693.52	J/molxK	1104.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391969&Units=SI

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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