Hydratropic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C15H18O2/c1-4-9-14(5-2)17-15(16)12(3)13-10-7-6-8-11-13/h6-8,10-12,14H,5H
InchiKey: UBDYWNRJPOSSMF-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: CC#CC(CC)OC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	151.83	kJ/mol	Joback Method
hf	-99.46	kJ/mol	Joback Method
hfus	27.51	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.135		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1620.00		NIST Webbook
tb	653.69	K	Joback Method
tc	881.56	K	Joback Method
tf	433.49	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.11	J/mol×K	653.69	Joback Method
cpg	522.13	J/mol×K	691.67	Joback Method
cpg	538.03	J/mol×K	729.65	Joback Method
cpg	552.86	J/mol×K	767.63	Joback Method
cpg	566.64	J/mol×K	805.61	Joback Method
cpg	579.41	J/mol×K	843.59	Joback Method
cpg	591.21	J/mol×K	881.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406956&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume