Hydratropic acid, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H24O2/c1-14(2)11-12-18(13-15(3)4)21-19(20)16(5)17-9-7-6-8-10-17/h6-10

InchiKey: XAUCKEXMIGASNZ-UHFFFAOYSA-N

Formula: C19H24O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)C(C)c1ccccc1

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	262.36	kJ/mol	Joback Method
hf	-71.66	kJ/mol	Joback Method
hfus	31.76	kJ/mol	Joback Method
hvap	69.72	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.328		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	741.33	K	Joback Method
tc	965.26	K	Joback Method
tf	447.85	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.72	J/mol×K	741.33	Joback Method
cpg	715.96	J/mol×K	778.65	Joback Method
cpg	732.95	J/mol×K	815.97	Joback Method
cpg	748.75	J/mol×K	853.30	Joback Method
cpg	763.40	J/mol×K	890.62	Joback Method
cpg	776.96	J/mol×K	927.94	Joback Method
cpg	789.49	J/mol×K	965.26	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=U406959&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