Hydratropic acid, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C22H32O2/c1-3-4-5-6-7-8-9-10-11-12-16-19-24-22(23)20(2)21-17-14-13-15-18
InchiKey: YHGYEFHSUCZMQR-UHFFFAOYSA-N
Formula: C22H32O2
SMILES: CCCCCCCCCCC#CCOC(=O)C(C)c1ccccc1
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	213.21	kJ/mol	Joback Method
hf	-238.66	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.868		Crippen Method
mcvol	295.920	ml/mol	McGowan Method
pc	1289.29	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	814.29	K	Joback Method
tc	1019.60	K	Joback Method
tf	527.38	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.52	J/mol×K	814.29	Joback Method
cpg	914.88	J/mol×K	848.51	Joback Method
cpg	932.07	J/mol×K	882.73	Joback Method
cpg	948.14	J/mol×K	916.95	Joback Method
cpg	963.13	J/mol×K	951.16	Joback Method
cpg	977.08	J/mol×K	985.38	Joback Method
cpg	990.05	J/mol×K	1019.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406961&Units=SI
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

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