Isovalerylphenylacetylene

Inchi: InChI=1S/C13H14O/c1-11(2)10-13(14)9-8-12-6-4-3-5-7-12/h3-7,11H,10H2,1-2H3
InchiKey: YSNUZHGXXPVDOQ-UHFFFAOYSA-N
Formula: C13H14O
SMILES: CC(C)CC(=O)C#Cc1ccccc1
Mol. weight [g/mol]: 186.25
CAS: 23566-47-4

Physical Properties

Property code	Value	Unit	Source
chl	-7207.80	kJ/mol	NIST Webbook
gf	242.43	kJ/mol	Joback Method
hf	79.32	kJ/mol	Joback Method
hfl	-41.80	kJ/mol	NIST Webbook
hfl	91.40 ± 6.00	kJ/mol	NIST Webbook
hfus	24.67	kJ/mol	Joback Method
hvap	55.32	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.653		Crippen Method
mcvol	163.240	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	585.95	K	Joback Method
tc	821.45	K	Joback Method
tf	403.72	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.80	J/mol×K	585.95	Joback Method
cpg	394.71	J/mol×K	625.20	Joback Method
cpg	409.55	J/mol×K	664.45	Joback Method
cpg	423.36	J/mol×K	703.70	Joback Method
cpg	436.21	J/mol×K	742.95	Joback Method
cpg	448.14	J/mol×K	782.20	Joback Method

cpg	459.20	J/mol×K	821.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23566474&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume