3,5-(CH3)2-C6H3-CCH

Inchi: InChI=1S/C10H10/c1-4-10-6-8(2)5-9(3)7-10/h1,5-7H,2-3H3
InchiKey: JVEFKVKLVXNSND-UHFFFAOYSA-N
Formula: C10H10
SMILES: C#Cc1cc(C)cc(C)c1
Mol. weight [g/mol]: 130.19
CAS: 6366-06-9

Physical Properties

Property code	Value	Unit	Source
affp	850.40	kJ/mol	NIST Webbook
basg	819.70	kJ/mol	NIST Webbook
gf	349.54	kJ/mol	Joback Method
hf	255.76	kJ/mol	Joback Method
hfus	17.89	kJ/mol	Joback Method
hvap	41.31	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.285		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	454.96	K	Joback Method
tc	678.23	K	Joback Method
tf	300.89	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.53	J/mol×K	454.96	Joback Method
cpg	240.15	J/mol×K	492.17	Joback Method
cpg	252.05	J/mol×K	529.38	Joback Method
cpg	263.25	J/mol×K	566.59	Joback Method
cpg	273.78	J/mol×K	603.81	Joback Method
cpg	283.68	J/mol×K	641.02	Joback Method
cpg	292.98	J/mol×K	678.23	Joback Method

Sources

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=C6366069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume