

Diphenylmethyl radical

Inchi:	InChI=1S/C13H11/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1-11H
InchiKey:	UIBVOXFCGWJCTC-UHFFFAOYSA-N
Formula:	C13H11
SMILES:	[CH](c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	167.23
CAS:	4471-17-4

Physical Properties

Property code	Value	Unit	Source
ea	1.36 ± 0.10	eV	NIST Webbook
ea	0.85 ± 0.26	eV	NIST Webbook
gf	333.34	kJ/mol	Joback Method
hf	211.94	kJ/mol	Joback Method
hfus	15.67	kJ/mol	Joback Method
hvap	48.55	kJ/mol	Joback Method
ie	7.30 ± 0.10	eV	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.287		Crippen Method
mcvol	144.360	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	549.06	K	Joback Method
tc	795.25	K	Joback Method
tf	290.48	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.32	J/mol×K	549.06	Joback Method
cpg	332.53	J/mol×K	590.09	Joback Method
cpg	347.33	J/mol×K	631.12	Joback Method
cpg	360.83	J/mol×K	672.15	Joback Method
cpg	373.17	J/mol×K	713.19	Joback Method
cpg	384.47	J/mol×K	754.22	Joback Method

cpg	394.86	J/mol×K	795.25	Joback Method
dvisc	0.0024492	Pa×s	290.48	Joback Method
dvisc	0.0014458	Pa×s	333.58	Joback Method
dvisc	0.0009629	Pa×s	376.67	Joback Method
dvisc	0.0006971	Pa×s	419.77	Joback Method
dvisc	0.0005360	Pa×s	462.87	Joback Method
dvisc	0.0004310	Pa×s	505.96	Joback Method
dvisc	0.0003586	Pa×s	549.06	Joback Method

Sources

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=C4471174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
ie:	Ionization energy
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

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