3-Methylbenzyl radical

Inchi: InChI=1S/C8H9/c1-7-4-3-5-8(2)6-7/h3-6H,1H2,2H3
InchiKey: GMRODCVDNXSFAA-UHFFFAOYSA-N
Formula: C8H9
SMILES: [CH2]c1cccc(C)c1
Mol. weight [g/mol]: 105.16
CAS: 2348-47-2

Physical Properties

Property code	Value	Unit	Source
ea	0.89 ± 0.15	eV	NIST Webbook
gf	171.64	kJ/mol	Joback Method
hf	72.42	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	36.19	kJ/mol	Joback Method
ie	7.65 ± 0.03	eV	NIST Webbook
ie	7.12 ± 0.02	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.177		Crippen Method
mcvol	97.670	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	413.40	K	Joback Method
tc	620.55	K	Joback Method
tf	235.23	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.79	J/mol×K	413.40	Joback Method
cpg	182.32	J/mol×K	447.92	Joback Method
cpg	193.08	J/mol×K	482.45	Joback Method
cpg	203.12	J/mol×K	516.97	Joback Method
cpg	212.48	J/mol×K	551.50	Joback Method
cpg	221.21	J/mol×K	586.02	Joback Method

cpg	229.36	J/mol×K	620.55	Joback Method
dvisc	0.0009752	Pa×s	235.23	Joback Method
dvisc	0.0007356	Pa×s	264.93	Joback Method
dvisc	0.0005873	Pa×s	294.62	Joback Method
dvisc	0.0004886	Pa×s	324.31	Joback Method
dvisc	0.0004193	Pa×s	354.01	Joback Method
dvisc	0.0003684	Pa×s	383.70	Joback Method
dvisc	0.0003298	Pa×s	413.40	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=C2348472&Units=SI

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