

Benzyl-d7 radical

Inchi:	InChI=1S/C7H7/c1-7-5-3-2-4-6-7/h2-6H,1H2/i1D2,2D,3D,4D,5D,6D
InchiKey:	SLRMQYXOBQWXCR-QMUWOJKRSA-N
Formula:	C7D7
SMILES:	[CH2]c1cccc1
Mol. weight [g/mol]:	98.17
CAS:	2154-55-4

Physical Properties

Property code	Value	Unit	Source
gf	172.85	kJ/mol	Joback Method
hf	104.53	kJ/mol	Joback Method
hfus	9.61	kJ/mol	Joback Method
hvap	33.31	kJ/mol	Joback Method
ie	7.24 ± 0.00	eV	NIST Webbook
log10ws	-1.57		Crippen Method
logp	1.869		Crippen Method
mcvol	83.580	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	385.54	K	Joback Method
tc	593.05	K	Joback Method
tf	211.44	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.68	J/molxK	385.54	Joback Method
cpg	143.52	J/molxK	420.12	Joback Method
cpg	153.56	J/molxK	454.71	Joback Method
cpg	162.85	J/molxK	489.29	Joback Method
cpg	171.44	J/molxK	523.88	Joback Method
cpg	179.38	J/molxK	558.46	Joback Method
cpg	186.73	J/molxK	593.05	Joback Method
dvisc	0.0010170	Paxs	211.44	Joback Method

dvisc	0.0007435	Paxs	240.46	Joback Method
dvisc	0.0005815	Paxs	269.47	Joback Method
dvisc	0.0004770	Paxs	298.49	Joback Method
dvisc	0.0004053	Paxs	327.51	Joback Method
dvisc	0.0003536	Paxs	356.52	Joback Method
dvisc	0.0003150	Paxs	385.54	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=C2154554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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