

9-Benzylfluorene

Inchi:	InChI=1S/C20H16/c1-2-8-15(9-3-1)14-20-18-12-6-4-10-16(18)17-11-5-7-13-19(17)20/h1-
InchiKey:	ZBQLAOVNDBNMFI-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	<chem>c1ccc(CC2c3ccccc3-c3ccccc32)cc1</chem>
Mol. weight [g/mol]:	256.34
CAS:	1572-46-9

Physical Properties

Property code	Value	Unit	Source
gf	520.44	kJ/mol	Joback Method
hf	315.64	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	67.84	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.042		Crippen Method
mcvol	210.520	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
tb	745.20	K	Joback Method
tc	1004.16	K	Joback Method
tf	444.44	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.43	J/molxK	745.20	Joback Method
cpg	597.53	J/molxK	788.36	Joback Method
cpg	613.28	J/molxK	831.52	Joback Method
cpg	627.89	J/molxK	874.68	Joback Method
cpg	641.56	J/molxK	917.84	Joback Method
cpg	654.48	J/molxK	961.00	Joback Method
cpg	666.84	J/molxK	1004.16	Joback Method
dvisc	0.0017300	Paxs	444.44	Joback Method
dvisc	0.0013013	Paxs	494.57	Joback Method

dvisc	0.0010314	Paxs	544.69	Joback Method
dvisc	0.0008502	Paxs	594.82	Joback Method
dvisc	0.0007222	Paxs	644.95	Joback Method
dvisc	0.0006281	Paxs	695.07	Joback Method
dvisc	0.0005566	Paxs	745.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1572469&Units=SI

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
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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