

2-CHLORO-6-FLUOROBENZYL CHLORIDE

Other names:	Benzene, 1-chloro-2-(chloromethyl)-3-fluoro-alpha,2-dichloro-6-fluorotoluene
Inchi:	InChI=1S/C7H5Cl2F/c8-4-5-6(9)2-1-3-7(5)10/h1-3H,4H2
InchiKey:	MJGOLNNLNQQIHR-UHFFFAOYSA-N
Formula:	C7H5Cl2F
SMILES:	Fc1cccc(Cl)c1CCl
Mol. weight [g/mol]:	179.02

Physical Properties

Property code	Value	Unit	Source
hfus	18.62	kJ/mol	Joback Method
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-3.14		Cheméo Relay (1.0)
logp	3.218		Crippen Method
mcvol	111.980	ml/mol	McGowan Method
tb	477.69	K	Cheméo Relay (1.0)
tf	312.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.08	J/mol×K	470.33	Joback Method
cpg	203.88	J/mol×K	506.49	Joback Method
cpg	212.14	J/mol×K	542.66	Joback Method
cpg	219.90	J/mol×K	578.82	Joback Method
cpg	227.17	J/mol×K	614.98	Joback Method
cpg	233.97	J/mol×K	651.14	Joback Method
cpg	240.32	J/mol×K	687.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55117152&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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