

4-Chloro-3-methylphenacyl bromide

Inchi:	InChI=1S/C9H8BrClO/c1-6-4-7(9(12)5-10)2-3-8(6)11/h2-4H,5H2,1H3
InchiKey:	LUCPZLPBUCDKQE-UHFFFAOYSA-N
Formula:	C9H8BrClO
SMILES:	Cc1cc(C(=O)CBr)ccc1Cl
Mol. weight [g/mol]:	247.52
CAS:	205178-80-9

Physical Properties

Property code	Value	Unit	Source
gf	-8.48	kJ/mol	Joback Method
hf	-117.49	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	56.79	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.226		Crippen Method
mcvol	145.220	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	599.42	K	Joback Method
tc	839.20	K	Joback Method
tf	382.30	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.29	J/molxK	599.42	Joback Method
cpg	335.08	J/molxK	799.23	Joback Method
cpg	327.45	J/molxK	759.27	Joback Method
cpg	319.20	J/molxK	719.31	Joback Method
cpg	310.28	J/molxK	679.35	Joback Method
cpg	300.66	J/molxK	639.38	Joback Method
cpg	342.13	J/molxK	839.20	Joback Method
dvisc	0.0002767	Paxs	599.42	Joback Method
dvisc	0.0003353	Paxs	563.23	Joback Method

dvisc	0.0004171	Paxs	527.05	Joback Method
dvisc	0.0005358	Paxs	490.86	Joback Method
dvisc	0.0007164	Paxs	454.67	Joback Method
dvisc	0.0010071	Paxs	418.49	Joback Method
dvisc	0.0015102	Paxs	382.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C205178809&Units=SI
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

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
mccvol:	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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