3-BROMO-5,5-DIMETHYL-CYCLOHEX-2-ENONE

Other names: 5,5-Dimethyl-3-bromocyclohex-2-enone
3-Bromo-5,5-dimethyl-cyclohex-2-enone
Inchi: InChI=1S/C8H11BrO/c1-8(2)4-6(9)3-7(10)5-8/h3H,4-5H2,1-2H3
InchiKey: LPZGJNIBSGPOED-UHFFFAOYSA-N
Formula: C8H11BrO
SMILES: CC1(C)CC(=O)C=C(Br)C1
Mol. weight [g/mol]: 203.08

Physical Properties

Property code	Value	Unit	Source
hfus	7.64	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-2.18		Cheméo Relay (1.0)
logp	2.654		Crippen Method
mcvol	127.490	ml/mol	McGowan Method
tb	499.71	K	Cheméo Relay (1.0)
tf	328.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.93	J/mol×K	540.35	Joback Method
cpg	285.19	J/mol×K	582.16	Joback Method
cpg	298.53	J/mol×K	623.98	Joback Method
cpg	311.08	J/mol×K	665.79	Joback Method
cpg	322.97	J/mol×K	707.60	Joback Method
cpg	334.32	J/mol×K	749.42	Joback Method
cpg	345.27	J/mol×K	791.23	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13271493&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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