

(E)-4-(3-Bromophenyl)-but-3-en-2-one

Inchi: InChI=1S/C10H9BrO/c1-8(12)5-6-9-3-2-4-10(11)7-9/h2-7H,1H3
InchiKey: QZOOCEEXEFIACMQ-UHFFFAOYSA-N
Formula: C10H9BrO
SMILES: CC(=O)C=Cc1cccc(Br)c1
Mol. weight [g/mol]: 225.08
CAS: 65300-30-3

Physical Properties

Property code	Value	Unit	Source
gf	101.72	kJ/mol	Joback Method
hf	6.30	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	3.051		Crippen Method
mcvol	142.770	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	584.05	K	Joback Method
tc	824.96	K	Joback Method
tf	346.05	K	Joback Method
vc	0.535	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.69	J/molxK	584.05	Joback Method
cpg	305.48	J/molxK	624.20	Joback Method
cpg	316.36	J/molxK	664.35	Joback Method
cpg	326.39	J/molxK	704.51	Joback Method
cpg	335.66	J/molxK	744.66	Joback Method
cpg	344.23	J/molxK	784.81	Joback Method
cpg	352.17	J/molxK	824.96	Joback Method
dvisc	0.0017851	Paxs	346.05	Joback Method

dvisc	0.0010639	Paxs	385.72	Joback Method
dvisc	0.0006984	Paxs	425.38	Joback Method
dvisc	0.0004925	Paxs	465.05	Joback Method
dvisc	0.0003670	Paxs	504.72	Joback Method
dvisc	0.0002854	Paxs	544.38	Joback Method
dvisc	0.0002297	Paxs	584.05	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=C65300303&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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