p-Bromophenyl heptyl ketone

Other names: p-Octanoylbromobenzene
Inchi: InChI=1S/C14H19BrO/c1-2-3-4-5-6-7-14(16)12-8-10-13(15)11-9-12/h8-11H,2-7H2,1H3
InchiKey: QMCHXDWPJPADAK-UHFFFAOYSA-N
Formula: C14H19BrO
SMILES: CCCCCCCC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 283.20
CAS: 7295-48-9

Physical Properties

Property code	Value	Unit	Source
gf	55.18	kJ/mol	Joback Method
hf	-193.48	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	62.88	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.992		Crippen Method
mcvol	203.430	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	671.41	K	Joback Method
tc	885.65	K	Joback Method
tf	396.21	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.18	J/mol×K	671.41	Joback Method
cpg	525.30	J/mol×K	707.12	Joback Method
cpg	539.47	J/mol×K	742.82	Joback Method
cpg	552.75	J/mol×K	778.53	Joback Method
cpg	565.18	J/mol×K	814.24	Joback Method
cpg	576.82	J/mol×K	849.94	Joback Method
cpg	587.71	J/mol×K	885.65	Joback Method
dvisc	0.0016043	Pa×s	396.21	Joback Method

dvisc	0.0009156	Pa×s	442.08	Joback Method
dvisc	0.0005807	Pa×s	487.94	Joback Method
dvisc	0.0003982	Pa×s	533.81	Joback Method
dvisc	0.0002899	Pa×s	579.68	Joback Method
dvisc	0.0002211	Pa×s	625.54	Joback Method
dvisc	0.0001750	Pa×s	671.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.50 ± 2.50	K	0.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C7295489&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume