

Octane, 2-bromo-, (.+/-.)-

Inchi:	InChI=1S/C8H17Br/c1-3-4-5-6-7-8(2)9/h8H,3-7H2,1-2H3
InchiKey:	FTJHYGJLHCGQHQ-UHFFFAOYSA-N
Formula:	C8H17Br
SMILES:	CCCCCCC(C)Br
Mol. weight [g/mol]:	193.12
CAS:	60251-57-2

Physical Properties

Property code	Value	Unit	Source
gf	28.36	kJ/mol	Joback Method
hf	-187.40	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.740		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	461.70	K	NIST Webbook
tc	633.14	K	Joback Method
tf	224.72	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.18	J/molxK	448.16	Joback Method
cpg	290.54	J/molxK	478.99	Joback Method
cpg	303.29	J/molxK	509.82	Joback Method
cpg	315.46	J/molxK	540.65	Joback Method
cpg	327.07	J/molxK	571.48	Joback Method
cpg	338.14	J/molxK	602.31	Joback Method
cpg	348.69	J/molxK	633.14	Joback Method
dvisc	0.0063866	Paxs	224.72	Joback Method
dvisc	0.0026570	Paxs	261.96	Joback Method

dvisc	0.0013751	Paxs	299.20	Joback Method
dvisc	0.0008234	Paxs	336.44	Joback Method
dvisc	0.0005461	Paxs	373.68	Joback Method
dvisc	0.0003902	Paxs	410.92	Joback Method
dvisc	0.0002948	Paxs	448.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	345.20	K	1.90	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60251572&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

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