Tricyclo[2.2.1.0^2^,^6]-heptane, 3-bromo-

Other names: Nortricyclyl bromide
Inchi: InChI=1S/C7H9Br/c8-7-3-1-4-5(2-3)6(4)7/h3-7H,1-2H2
InchiKey: RDIUINMODIQXGA-UHFFFAOYSA-N
Formula: C7H9Br
SMILES: BrC1C2CC3C(C2)C13
Mol. weight [g/mol]: 173.05
CAS: 695-02-3

Physical Properties

Property code	Value	Unit	Source
gf	213.41	kJ/mol	Joback Method
hf	28.56	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	36.39	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.036		Crippen Method
mcvol	94.410	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	428.06	K	Joback Method
tc	642.63	K	Joback Method
tf	280.83	K	Joback Method
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.78	J/mol×K	428.06	Joback Method
cpg	256.02	J/mol×K	606.87	Joback Method
cpg	245.71	J/mol×K	571.11	Joback Method
cpg	234.43	J/mol×K	535.34	Joback Method
cpg	222.10	J/mol×K	499.58	Joback Method
cpg	208.58	J/mol×K	463.82	Joback Method
cpg	265.50	J/mol×K	642.63	Joback Method
dvisc	0.0018989	Pa×s	428.06	Joback Method

dvisc	0.0015978	Pa×s	403.52	Joback Method
dvisc	0.0013147	Pa×s	378.98	Joback Method
dvisc	0.0010530	Pa×s	354.44	Joback Method
dvisc	0.0008159	Pa×s	329.91	Joback Method
dvisc	0.0006069	Pa×s	305.37	Joback Method
dvisc	0.0004286	Pa×s	280.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.00 ± 1.00	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C695023&Units=SI
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

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