Octane, 2-bromo-3-(trichloromethyl), erythro

Inchi: InChI=1S/C9H16BrCl3/c1-3-4-5-6-8(7(2)10)9(11,12)13/h7-8H,3-6H2,1-2H3/t7-,8+/m1/s1
InchiKey: LGJUZIWUDCVORF-SFYZADRCSA-N
Formula: C9H16BrCl3
SMILES: CCCCCC(C(C)Br)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 310.49

Physical Properties

Property code	Value	Unit	Source
gf	1.39	kJ/mol	Joback Method
hf	-269.29	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	53.15	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.337		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1515.00		NIST Webbook
tb	579.66	K	Joback Method
tc	793.91	K	Joback Method
tf	313.17	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.74	J/mol×K	579.66	Joback Method
cpg	422.00	J/mol×K	615.37	Joback Method
cpg	434.34	J/mol×K	651.08	Joback Method
cpg	445.84	J/mol×K	686.78	Joback Method
cpg	456.56	J/mol×K	722.49	Joback Method
cpg	466.56	J/mol×K	758.20	Joback Method
cpg	475.89	J/mol×K	793.91	Joback Method
dvisc	0.0053032	Pa×s	313.17	Joback Method
dvisc	0.0021530	Pa×s	357.59	Joback Method

dvisc	0.0010668	Pa×s	402.00	Joback Method
dvisc	0.0006078	Pa×s	446.42	Joback Method
dvisc	0.0003834	Pa×s	490.83	Joback Method
dvisc	0.0002611	Pa×s	535.25	Joback Method
dvisc	0.0001886	Pa×s	579.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515474&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume