rac-2,3-Dichlorobutane

Inchi: InChI=1S/C4H8Cl2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey: RMISVOPUIFJTEO-IMJSIDKUSA-N
Formula: C4H8Cl2
SMILES: CC(Cl)C(C)Cl
Mol. weight [g/mol]: 127.01

Physical Properties

Property code	Value	Unit	Source
gf	-45.94	kJ/mol	Joback Method
hf	-167.93	kJ/mol	Joback Method
hfus	7.46	kJ/mol	Joback Method
hvap	32.49	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.241		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	903.00		NIST Webbook
tb	364.90	K	Joback Method
tc	555.91	K	Joback Method
tf	164.68	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.51	J/mol×K	364.90	Joback Method
cpg	149.43	J/mol×K	396.73	Joback Method
cpg	157.00	J/mol×K	428.57	Joback Method
cpg	164.21	J/mol×K	460.40	Joback Method
cpg	171.09	J/mol×K	492.24	Joback Method
cpg	177.64	J/mol×K	524.07	Joback Method
cpg	183.87	J/mol×K	555.91	Joback Method
dvisc	0.0130687	Pa×s	164.68	Joback Method
dvisc	0.0042176	Pa×s	198.05	Joback Method

dvisc	0.0018860	Pa×s	231.42	Joback Method
dvisc	0.0010331	Pa×s	264.79	Joback Method
dvisc	0.0006475	Pa×s	298.16	Joback Method
dvisc	0.0004458	Pa×s	331.53	Joback Method
dvisc	0.0003287	Pa×s	364.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R597243&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

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