Trans-1-butyl-2-methylcyclopropane

Other names: 1-Butyl-2-methylcyclopropane, (E)-
Inchi: InChI=1S/C8H16/c1-3-4-5-8-6-7(8)2/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey: IWTBNPKBPXCCIV-YUMQZZPRSA-N
Formula: C8H16
SMILES: CCCC[C@@H]1C[C@H]1C
Mol. weight [g/mol]: 112.22

Physical Properties

Property code	Value	Unit	Source
af	0.3089		Cheméo Relay (1.0)
gf	69.52	kJ/mol	Joback Method
hf	-77.38	kJ/mol	Cheméo Relay (1.0)
hfus	15.68	kJ/mol	Joback Method
hvap	37.98	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	790.00		NIST Webbook
tb	386.92	K	Cheméo Relay (1.0)
tc	593.03	K	Cheméo Relay (1.0)
tf	142.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.48	J/mol×K	384.51	Joback Method
cpg	295.82	J/mol×K	561.42	Joback Method
cpg	284.10	J/mol×K	531.93	Joback Method
cpg	271.82	J/mol×K	502.45	Joback Method
cpg	258.93	J/mol×K	472.96	Joback Method
cpg	245.43	J/mol×K	443.48	Joback Method
cpg	231.29	J/mol×K	413.99	Joback Method
dvisc	0.0004205	Pa×s	289.06	Joback Method

dvisc	0.0003249	Pa×s	384.51	Joback Method
dvisc	0.0003486	Pa×s	352.69	Joback Method
dvisc	0.0003793	Pa×s	320.88	Joback Method
dvisc	0.0007016	Pa×s	193.62	Joback Method
dvisc	0.0004781	Pa×s	257.25	Joback Method
dvisc	0.0005637	Pa×s	225.44	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38851706&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie: Ionization energy
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

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