1-Butene, 3-methyl-2-(1-methylethyl)

Other names: 2-Isopropyl-3-methylbut-1-ene
3-methyl-2-(1-methylethyl)-1-butene
Inchi: InChI=1S/C8H16/c1-6(2)8(5)7(3)4/h6-7H,5H2,1-4H3
InchiKey: GIBPFTYFAOOKOV-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C(C)C)C(C)C
Mol. weight [g/mol]: 112.21
CAS: 111823-35-9

Physical Properties

Property code	Value	Unit	Source
gf	90.89	kJ/mol	Joback Method
hf	-103.37	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	32.04	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.855		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	720.30		NIST Webbook
rinpol	720.30		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	720.00		NIST Webbook
rinpol	710.50		NIST Webbook
rinpol	708.50		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	709.30		NIST Webbook
tb	378.12	K	Joback Method
tc	556.32	K	Joback Method
tf	134.20	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.46	J/mol×K	378.12	Joback Method
cpg	230.96	J/mol×K	407.82	Joback Method
cpg	243.91	J/mol×K	437.52	Joback Method
cpg	256.31	J/mol×K	467.22	Joback Method
cpg	268.18	J/mol×K	496.92	Joback Method
cpg	279.54	J/mol×K	526.62	Joback Method
cpg	290.40	J/mol×K	556.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111823359&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol339.mol

Legend

cpg: Ideal gas heat capacity
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