2-Ethyl-3,3-dimethylbut-1-ene

Other names: 1-Butene, 2-ethyl-3,3-dimethyl
3,3-Dimethyl-2-ethyl-1-butene
Inchi: InChI=1S/C8H16/c1-6-7(2)8(3,4)5/h2,6H2,1,3-5H3
InchiKey: KQRPZENSXZIOQO-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(CC)C(C)(C)C
Mol. weight [g/mol]: 112.21
CAS: 18231-53-3

Physical Properties

Property code	Value	Unit	Source
gf	98.61	kJ/mol	Joback Method
hf	-101.56	kJ/mol	Joback Method
hfus	6.47	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	739.60		NIST Webbook
rinpol	739.60		NIST Webbook
rinpol	729.50		NIST Webbook
rinpol	731.00		NIST Webbook
tb	383.75 ± 0.40	K	NIST Webbook
tb	390.35 ± 0.30	K	NIST Webbook
tc	557.27	K	Joback Method
tf	166.62	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/mol×K	375.77	Joback Method
cpg	232.95	J/mol×K	406.02	Joback Method

cpg	246.58	J/mol×K	436.27	Joback Method
cpg	259.50	J/mol×K	466.52	Joback Method
cpg	271.77	J/mol×K	496.77	Joback Method
cpg	283.40	J/mol×K	527.02	Joback Method
cpg	294.42	J/mol×K	557.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29372e+01
Coeff. B	-2.68757e+03
Coeff. C	-6.72810e+01
Temperature range (K), min.	279.74
Temperature range (K), max.	419.72

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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/mol340.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18231533&Units=SI

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume