3-Ethyl-1,1-dimethylcyclopentane

Other names: 3-Ethyl-1,1-dimethylcyclopentane
Inchi: InChI=1S/C9H18/c1-4-8-5-6-9(2,3)7-8/h8H,4-7H2,1-3H3
InchiKey: WXHYOGXBESCULU-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCC1CCC(C)(C)C1
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
hfus	7.77	kJ/mol	Joback Method
hvap	41.36	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
rinpol	821.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	824.60		NIST Webbook
rinpol	830.20		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	828.60		NIST Webbook
tb	401.60	K	Cheméo Relay (1.0)
tf	160.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.68	J/mol×K	416.17	Joback Method
cpg	275.18	J/mol×K	449.38	Joback Method
cpg	292.53	J/mol×K	482.58	Joback Method

cpg	308.81	J/mol×K	515.79	Joback Method
cpg	324.12	J/mol×K	548.99	Joback Method
cpg	338.53	J/mol×K	582.20	Joback Method
cpg	352.15	J/mol×K	615.40	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=C62016619&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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point