

trans-1-Butyl-2-ethylcyclopentane

Inchi: InChI=1S/C11H22/c1-3-5-7-11-9-6-8-10(11)4-2/h10-11H,3-9H2,1-2H3/t10-,11-/m0/s1
InchiKey: YJMFUCKUZMNZLY-QWRGUYRKSA-N
Formula: C11H22
SMILES: CCCCC1CCCC1CC
Mol. weight [g/mol]: 154.29

Physical Properties

Property code	Value	Unit	Source
gf	70.58	kJ/mol	Joback Method
hf	-230.23	kJ/mol	Joback Method
hfus	19.25	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	4.003		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1083.00		NIST Webbook
rinpol	1087.00		NIST Webbook
tb	461.69	K	Joback Method
tc	648.77	K	Joback Method
tf	220.39	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.22	J/mol×K	461.69	Joback Method
cpg	435.30	J/mol×K	617.59	Joback Method
cpg	419.15	J/mol×K	586.41	Joback Method
cpg	402.19	J/mol×K	555.23	Joback Method
cpg	384.40	J/mol×K	524.05	Joback Method
cpg	365.75	J/mol×K	492.87	Joback Method
cpg	450.67	J/mol×K	648.77	Joback Method
dvisc	0.0003027	Pa×s	461.69	Joback Method

dvisc	0.0003729	Pa×s	421.47	Joback Method
dvisc	0.0004801	Pa×s	381.26	Joback Method
dvisc	0.0006560	Pa×s	341.04	Joback Method
dvisc	0.0009745	Pa×s	300.82	Joback Method
dvisc	0.0016355	Pa×s	260.61	Joback Method
dvisc	0.0033159	Pa×s	220.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143698&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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