Cyclohexane, 2-butyl-1,1,3-trimethyl-

Other names:	1,1,3-Trimethyl-2-butyl-cyclohexane
	2-Butyl-1,1,3-trimethylcyclohexane
Inchi:	InChI=1S/C13H26/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h11-12H,5-10H2,1-4H3
InchiKey:	PUUCZCJOATUHNE-UHFFFAOYSA-N
Formula:	C13H26
SMILES:	CCCCC1C(C)CCCC1(C)C
Mol. weight [g/mol]:	182.35
CAS:	54676-39-0

Physical Properties

Property code	Value	Unit	Source
gf	62.12	kJ/mol	Joback Method
hf	-282.77	kJ/mol	Joback Method
hfus	17.11	kJ/mol	Joback Method
hvap	43.19	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.639		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1228.00		NIST Webbook
tb	507.29	K	Joback Method
tc	704.36	K	Joback Method
tf	259.07	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.22	J/mol×K	507.29	Joback Method
cpg	467.63	J/mol×K	540.14	Joback Method
cpg	488.86	J/mol×K	572.98	Joback Method
cpg	509.00	J/mol×K	605.83	Joback Method
cpg	528.12	J/mol×K	638.67	Joback Method
cpg	546.32	J/mol×K	671.52	Joback Method

cpg	563.67	J/mol×K	704.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48084e+01
Coeff. B	-4.28856e+03
Coeff. C	-8.30740e+01
Temperature range (K), min.	378.41
Temperature range (K), max.	534.65

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54676390&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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