

trans-1-butyl-2-methylcyclopentane

Other names:	trans-1-Butyl-2-methylcyclopentane
Inchi:	InChI=1S/C10H20/c1-3-4-7-10-8-5-6-9(10)2/h9-10H,3-8H2,1-2H3
InchiKey:	CBGQSQYVGVKUCW-UWVGGRQHSA-N
Formula:	C10H20
SMILES:	CCCCC1CCCC1C
Mol. weight [g/mol]:	140.27
CAS:	53366-35-1

Physical Properties

Property code	Value	Unit	Source
af	0.3467		Cheméo Relay (1.0)
gf	62.16	kJ/mol	Joback Method
hf	-190.47	kJ/mol	Cheméo Relay (1.0)
hfus	16.66	kJ/mol	Joback Method
hvap	47.14	kJ/mol	Cheméo Relay (1.0)
ie	9.35	eV	Cheméo Relay (1.0)
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	442.60 ± 1.50	K	NIST Webbook
tc	634.42	K	Cheméo Relay (1.0)
tf	167.34	K	Cheméo Relay (1.0)
vc	0.509	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.00	J/mol×K	438.81	Joback Method
cpg	318.72	J/mol×K	470.30	Joback Method
cpg	336.60	J/mol×K	501.79	Joback Method
cpg	353.67	J/mol×K	533.28	Joback Method
cpg	369.93	J/mol×K	564.77	Joback Method
cpg	385.42	J/mol×K	596.26	Joback Method
cpg	400.16	J/mol×K	627.75	Joback Method

dvisc	0.0030012	Pa×s	209.12	Joback Method
dvisc	0.0015247	Pa×s	247.40	Joback Method
dvisc	0.0009287	Pa×s	285.68	Joback Method
dvisc	0.0006360	Pa×s	323.97	Joback Method
dvisc	0.0004719	Pa×s	362.25	Joback Method
dvisc	0.0003706	Pa×s	400.53	Joback Method
dvisc	0.0003036	Pa×s	438.81	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53366351&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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