

Ethyl trans-3-t-butylcyclobutanecarboxylate

Inchi:	InChI=1S/C11H20O2/c1-5-13-10(12)8-6-9(7-8)11(2,3)4/h8-9H,5-7H2,1-4H3/t8-,9-
InchiKey:	NDKCMUOLZJVCTI-KYZUINATSA-N
Formula:	C11H20O2
SMILES:	CCOC(=O)C1CC(C(C)(C)C)C1
Mol. weight [g/mol]:	184.28
CAS:	14924-52-8

Physical Properties

Property code	Value	Unit	Source
gf	-148.40	kJ/mol	Joback Method
hf	-477.62	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.622		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
tb	530.48	K	Joback Method
tc	730.66	K	Joback Method
tf	298.49	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.87	J/molxK	530.48	Joback Method
cpg	487.27	J/molxK	697.30	Joback Method
cpg	472.84	J/molxK	663.94	Joback Method
cpg	457.52	J/molxK	630.57	Joback Method
cpg	441.28	J/molxK	597.21	Joback Method
cpg	424.08	J/molxK	563.84	Joback Method
cpg	500.85	J/molxK	730.66	Joback Method
dvisc	0.0003579	Paxs	530.48	Joback Method
dvisc	0.0004407	Paxs	491.81	Joback Method

dvisc	0.0005624	Paxs	453.15	Joback Method
dvisc	0.0007510	Paxs	414.49	Joback Method
dvisc	0.0010643	Paxs	375.82	Joback Method
dvisc	0.0016340	Paxs	337.16	Joback Method
dvisc	0.0028032	Paxs	298.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14924528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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