methyl 3,3-dimethylcyclohexanecarboxylate

Inchi: InChI=1S/C10H18O2/c1-10(2)6-4-5-8(7-10)9(11)12-3/h8H,4-7H2,1-3H3
InchiKey: BSBYCHDVFUBBOV-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: COC(=O)C1CCCC(C)(C)C1
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-189.35	kJ/mol	Joback Method
hf	-445.31	kJ/mol	Joback Method
hfus	11.05	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.376		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
tb	519.61	K	Joback Method
tc	733.33	K	Joback Method
tf	301.66	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.82	J/mol×K	519.61	Joback Method
cpg	374.01	J/mol×K	555.23	Joback Method
cpg	391.16	J/mol×K	590.85	Joback Method
cpg	407.36	J/mol×K	626.47	Joback Method
cpg	422.69	J/mol×K	662.09	Joback Method
cpg	437.25	J/mol×K	697.71	Joback Method
cpg	451.12	J/mol×K	733.33	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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