Cyclohexanecarboxylic acid, 3-methylbutyl ester

Other names: isopentyl cyclohexanecarboxylate
Inchi: InChI=1S/C12H22O2/c1-10(2)8-9-14-12(13)11-6-4-3-5-7-11/h10-11H,3-9H2,1-2H3
InchiKey: VLALRUKXGDUQFX-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CC(C)CCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 198.30
CAS: 25183-19-1

Physical Properties

Property code	Value	Unit	Source
gf	-161.75	kJ/mol	Joback Method
hf	-486.77	kJ/mol	Joback Method
hfus	17.93	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.156		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
tb	569.36	K	Joback Method
tc	772.89	K	Joback Method
tf	289.54	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.79	J/mol×K	569.36	Joback Method
cpg	542.39	J/mol×K	738.97	Joback Method
cpg	526.84	J/mol×K	705.05	Joback Method
cpg	510.33	J/mol×K	671.13	Joback Method
cpg	492.83	J/mol×K	637.20	Joback Method
cpg	474.32	J/mol×K	603.28	Joback Method

cpg	556.98	J/mol×K	772.89	Joback Method
dvisc	0.0001888	Pa×s	569.36	Joback Method
dvisc	0.0002571	Pa×s	522.72	Joback Method
dvisc	0.0003719	Pa×s	476.09	Joback Method
dvisc	0.0005831	Pa×s	429.45	Joback Method
dvisc	0.0010198	Pa×s	382.81	Joback Method
dvisc	0.0020829	Pa×s	336.18	Joback Method
dvisc	0.0053547	Pa×s	289.54	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25183191&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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