

Cyclohexanecarboxylic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H20O2/c1-11-8-12(2)10-14(9-11)17-15(16)13-6-4-3-5-7-13/h8-10,13H,3-7H
InchiKey: ZJPBGWIGOQJVBM-UHFFFAOYSA-N
Formula: C15H20O2
SMILES: Cc1cc(C)cc(OC(=O)C2CCCCC2)c1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	-40.90	kJ/mol	Joback Method
hf	-329.82	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.789		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1796.00		NIST Webbook
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tb	675.08	K	Joback Method
tc	907.35	K	Joback Method
tf	389.81	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.40	J/molxK	675.08	Joback Method
cpg	622.09	J/molxK	868.64	Joback Method
cpg	607.93	J/molxK	829.93	Joback Method
cpg	592.51	J/molxK	791.21	Joback Method
cpg	575.80	J/molxK	752.50	Joback Method
cpg	557.78	J/molxK	713.79	Joback Method
cpg	635.02	J/molxK	907.35	Joback Method
dvisc	0.0001423	Paxs	675.08	Joback Method

dvisc	0.0001811	Paxs	627.54	Joback Method
dvisc	0.0002397	Paxs	579.99	Joback Method
dvisc	0.0003335	Paxs	532.45	Joback Method
dvisc	0.0004952	Paxs	484.90	Joback Method
dvisc	0.0008012	Paxs	437.36	Joback Method
dvisc	0.0014577	Paxs	389.81	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=U307704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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