

Cyclobutanecarboxylic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H10Cl2O2/c12-9-5-4-8(6-10(9)13)15-11(14)7-2-1-3-7/h4-7H,1-3H2
InchiKey: APPODQFYNHYRBW-UHFFFAOYSA-N
Formula: C11H10Cl2O2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)C1CCC1
Mol. weight [g/mol]: 245.10

Physical Properties

Property code	Value	Unit	Source
gf	-74.24	kJ/mol	Joback Method
hf	-266.42	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	61.69	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.699		Crippen Method
mcvol	163.150	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	1738.00		NIST Webbook
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tb	649.88	K	Joback Method
tc	891.96	K	Joback Method
tf	411.61	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.81	J/mol×K	649.88	Joback Method
cpg	439.53	J/mol×K	851.61	Joback Method
cpg	430.02	J/mol×K	811.27	Joback Method
cpg	419.64	J/mol×K	770.92	Joback Method
cpg	408.34	J/mol×K	730.57	Joback Method
cpg	396.08	J/mol×K	690.23	Joback Method
cpg	448.22	J/mol×K	891.96	Joback Method
dvisc	0.0003410	Pa×s	649.88	Joback Method

dvisc	0.0004037	Pa×s	610.17	Joback Method
dvisc	0.0004893	Pa×s	570.46	Joback Method
dvisc	0.0006103	Pa×s	530.75	Joback Method
dvisc	0.0007891	Pa×s	491.03	Joback Method
dvisc	0.0010673	Pa×s	451.32	Joback Method
dvisc	0.0015303	Pa×s	411.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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