

2-Methylvaleric acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C12H14Cl2O2/c1-3-4-8(2)12(15)16-9-5-6-10(13)11(14)7-9/h5-8H,3-4H2,1-2H3
InchiKey:	VOBRYODGNSVURY-UHFFFAOYSA-N
Formula:	C12H14Cl2O2
SMILES:	CCCC(C)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	261.14

Physical Properties

Property code	Value	Unit	Source
gf	-116.91	kJ/mol	Joback Method
hf	-358.98	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.335		Crippen Method
mvol	188.100	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1766.00		NIST Webbook
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tb	661.31	K	Joback Method
tc	880.74	K	Joback Method
tf	393.46	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.80	J/molxK	661.31	Joback Method
cpg	504.46	J/molxK	844.17	Joback Method
cpg	494.53	J/molxK	807.59	Joback Method
cpg	483.81	J/molxK	771.02	Joback Method
cpg	472.30	J/molxK	734.45	Joback Method
cpg	459.97	J/molxK	697.88	Joback Method
cpg	513.62	J/molxK	880.74	Joback Method
dvisc	0.0001486	Paxs	661.31	Joback Method

dvisc	0.0001874	Paxs	616.67	Joback Method
dvisc	0.0002451	Paxs	572.03	Joback Method
dvisc	0.0003354	Paxs	527.38	Joback Method
dvisc	0.0004865	Paxs	482.74	Joback Method
dvisc	0.0007610	Paxs	438.10	Joback Method
dvisc	0.0013178	Paxs	393.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357764&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	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
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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