Valeric acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H12Cl2O2/c1-2-3-4-11(14)15-8-5-6-9(12)10(13)7-8/h5-7H,2-4H2,1H3
InchiKey: YNABTDZJUAFPIV-UHFFFAOYSA-N
Formula: C11H12Cl2O2
SMILES: CCCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 247.12

Physical Properties

Property code	Value	Unit	Source
gf	-122.89	kJ/mol	Joback Method
hf	-333.06	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.089		Crippen Method
mcvol	174.010	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	638.87	K	Joback Method
tc	857.81	K	Joback Method
tf	397.19	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.95	J/mol×K	638.87	Joback Method
cpg	450.59	J/mol×K	821.32	Joback Method
cpg	441.31	J/mol×K	784.83	Joback Method
cpg	431.31	J/mol×K	748.34	Joback Method
cpg	420.60	J/mol×K	711.85	Joback Method
cpg	409.15	J/mol×K	675.36	Joback Method
cpg	459.17	J/mol×K	857.81	Joback Method
dvisc	0.0001786	Pa×s	638.87	Joback Method

dvisc	0.0002202	Pa×s	598.59	Joback Method
dvisc	0.0002798	Pa×s	558.31	Joback Method
dvisc	0.0003691	Pa×s	518.03	Joback Method
dvisc	0.0005101	Pa×s	477.75	Joback Method
dvisc	0.0007483	Pa×s	437.47	Joback Method
dvisc	0.0011863	Pa×s	397.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307988&Units=SI

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