2-Ethylbutyric acid, 2,4-dichloro-6-formylphenyl ester

Inchi: InChI=1S/C13H14Cl2O3/c1-3-8(4-2)13(17)18-12-9(7-16)5-10(14)6-11(12)15/h5-8H,3-4H

InchiKey: MAVNNZQOAIZABL-UHFFFAOYSA-N

Formula: C13H14Cl2O3

SMILES: CCC(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 289.15

Physical Properties

Property code	Value	Unit	Source
gf	-217.64	kJ/mol	Joback Method
hf	-476.67	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	73.05	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.148		Crippen Method
mcvol	203.760	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	737.83	K	Joback Method
tc	956.33	K	Joback Method
tf	459.25	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.19	J/mol×K	737.83	Joback Method
cpg	561.47	J/mol×K	919.91	Joback Method
cpg	552.82	J/mol×K	883.50	Joback Method
cpg	543.39	J/mol×K	847.08	Joback Method
cpg	533.15	J/mol×K	810.66	Joback Method
cpg	522.09	J/mol×K	774.25	Joback Method
cpg	569.33	J/mol×K	956.33	Joback Method
dvisc	0.0001471	Pa×s	737.83	Joback Method

dvisc	0.0001823	Pa×s	691.40	Joback Method
dvisc	0.0002329	Pa×s	644.97	Joback Method
dvisc	0.0003092	Pa×s	598.54	Joback Method
dvisc	0.0004305	Pa×s	552.11	Joback Method
dvisc	0.0006369	Pa×s	505.68	Joback Method
dvisc	0.0010200	Pa×s	459.25	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=U370077&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