2-Ethylbutyric acid, 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C16H16Cl2O2/c1-3-10(4-2)16(19)20-15-12-8-6-5-7-11(12)13(17)9-14(15)18/h5

InchiKey: XJERCQMCZLVUQI-UHFFFAOYSA-N

Formula: C16H16Cl2O2

SMILES: CCC(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 311.20

Physical Properties

Property code	Value	Unit	Source
gf	13.79	kJ/mol	Joback Method
hf	-261.94	kJ/mol	Joback Method
hfus	34.75	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.488		Crippen Method
mcvol	225.000	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2263.00		NIST Webbook
tb	776.79	K	Joback Method
tc	1006.27	K	Joback Method
tf	483.76	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.17	J/mol×K	776.79	Joback Method
cpg	599.40	J/mol×K	815.04	Joback Method
cpg	611.67	J/mol×K	853.28	Joback Method
cpg	623.06	J/mol×K	891.53	Joback Method
cpg	633.60	J/mol×K	929.78	Joback Method
cpg	643.36	J/mol×K	968.03	Joback Method
cpg	652.39	J/mol×K	1006.27	Joback Method
dvisc	0.0009259	Pa×s	483.76	Joback Method
dvisc	0.0006163	Pa×s	532.60	Joback Method

dvisc	0.0004392	Pa×s	581.44	Joback Method
dvisc	0.0003299	Pa×s	630.27	Joback Method
dvisc	0.0002582	Pa×s	679.11	Joback Method
dvisc	0.0002088	Pa×s	727.95	Joback Method
dvisc	0.0001735	Pa×s	776.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370061&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

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