Formic acid, (2,6-dichlorophenyl)metyl ester

Inchi: InChI=1S/C8H6Cl2O2/c9-7-2-1-3-8(10)6(7)4-12-5-11/h1-3,5H,4H2
InchiKey: DHBLRKXMKKQDBC-UHFFFAOYSA-N
Formula: C8H6Cl2O2
SMILES: O=COCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 205.04

Physical Properties

Property code	Value	Unit	Source
gf	-118.75	kJ/mol	Joback Method
hf	-244.14	kJ/mol	Joback Method
hfus	21.61	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.666		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	1449.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	565.02	K	Joback Method
tc	791.18	K	Joback Method
tf	355.45	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.21	J/mol×K	565.02	Joback Method
cpg	300.37	J/mol×K	753.49	Joback Method
cpg	293.41	J/mol×K	715.79	Joback Method
cpg	285.92	J/mol×K	678.10	Joback Method
cpg	277.90	J/mol×K	640.41	Joback Method
cpg	269.33	J/mol×K	602.71	Joback Method
cpg	306.80	J/mol×K	791.18	Joback Method
dvisc	0.0002610	Pa×s	565.02	Joback Method

dvisc	0.0003164	Pa×s	530.09	Joback Method
dvisc	0.0003942	Pa×s	495.16	Joback Method
dvisc	0.0005078	Pa×s	460.24	Joback Method
dvisc	0.0006819	Pa×s	425.31	Joback Method
dvisc	0.0009653	Pa×s	390.38	Joback Method
dvisc	0.0014631	Pa×s	355.45	Joback Method

Sources

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=U368897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/68-657-8/Formic-acid-2-6-dichlorophenyl-metyl-ester.pdf
Generated by Cheméo on 2024-10-12 06:57:59.69248223 +0000 UTC m=+3297142.329451479.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.