3-Phenylpropionic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C15H12Cl2O2/c16-13-8-7-12(10-14(13)17)19-15(18)9-6-11-4-2-1-3-5-11/h1-5,

InchiKey: FQOCOCXQBBVPNZ-UHFFFAOYSA-N

Formula: C15H12Cl2O2

SMILES: O=C(CCc1ccccc1)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 295.16

Physical Properties

Property code	Value	Unit	Source
gf	23.20	kJ/mol	Joback Method
hf	-179.09	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.532		Crippen Method
mcvol	206.610	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	2177.00		NIST Webbook
tb	757.07	K	Joback Method
tc	1001.10	K	Joback Method
tf	468.69	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.29	J/mol×K	757.07	Joback Method
cpg	566.61	J/mol×K	960.43	Joback Method
cpg	557.99	J/mol×K	919.75	Joback Method
cpg	548.39	J/mol×K	879.08	Joback Method
cpg	537.77	J/mol×K	838.41	Joback Method
cpg	526.09	J/mol×K	797.74	Joback Method
cpg	574.32	J/mol×K	1001.10	Joback Method
dvisc	0.0001143	Pa×s	757.07	Joback Method
dvisc	0.0001416	Pa×s	709.01	Joback Method

dvisc	0.0001811	Pa×s	660.94	Joback Method
dvisc	0.0002408	Pa×s	612.88	Joback Method
dvisc	0.0003359	Pa×s	564.82	Joback Method
dvisc	0.0004986	Pa×s	516.75	Joback Method
dvisc	0.0008024	Pa×s	468.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307785&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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