2-(Methylthio)benzoic acid, 2-(2-chlorophenoxy)ethyl ester

Inchi: InChI=1S/C16H15ClO3S/c1-21-15-9-5-2-6-12(15)16(18)20-11-10-19-14-8-4-3-7-13(14)17

InchiKey: BIDIXAGHTAKBEZ-UHFFFAOYSA-N

Formula: C16H15ClO3S

SMILES: CSc1ccccc1C(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 322.81

Physical Properties

Property code	Value	Unit	Source
gf	-28.33	kJ/mol	Joback Method
hf	-274.34	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.298		Crippen Method
mcvol	230.680	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2638.00		NIST Webbook
tb	833.72	K	Joback Method
tc	1081.21	K	Joback Method
tf	506.67	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.36	J/mol×K	833.72	Joback Method
cpg	632.12	J/mol×K	874.97	Joback Method
cpg	643.51	J/mol×K	916.22	Joback Method
cpg	653.56	J/mol×K	957.47	Joback Method
cpg	662.28	J/mol×K	998.72	Joback Method
cpg	669.69	J/mol×K	1039.97	Joback Method
cpg	675.81	J/mol×K	1081.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375051&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
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