4-(Methylthio)benzoic acid, 2-(2-chlorophenethyl) ester

Inchi: InChI=1S/C16H15ClO2S/c1-20-14-8-6-13(7-9-14)16(18)19-11-10-12-4-2-3-5-15(12)17/h2

InchiKey: LSAHCSSANLGVFJ-UHFFFAOYSA-N

Formula: C16H15ClO2S

SMILES: CSc1ccc(C(=O)OCCc2ccccc2Cl)cc1

Mol. weight [g/mol]: 306.81

Physical Properties

Property code	Value	Unit	Source
gf	76.67	kJ/mol	Joback Method
hf	-142.12	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.461		Crippen Method
mcvol	224.810	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	811.30	K	Joback Method
tc	1062.43	K	Joback Method
tf	484.44	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.82	J/mol×K	811.30	Joback Method
cpg	607.20	J/mol×K	853.15	Joback Method
cpg	619.26	J/mol×K	895.01	Joback Method
cpg	630.06	J/mol×K	936.86	Joback Method
cpg	639.62	J/mol×K	978.72	Joback Method
cpg	648.01	J/mol×K	1020.57	Joback Method
cpg	655.25	J/mol×K	1062.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375065&Units=SI

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