4-Methoxybenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C16H23ClO3/c1-19-15-10-8-14(9-11-15)16(18)20-13-7-5-3-2-4-6-12-17/h8-11H
InchiKey: NBGBVTBBAOFRQV-UHFFFAOYSA-N
Formula: C16H23ClO3
SMILES: COc1ccc(C(=O)OCCCCCCCCCCl)cc1
Mol. weight [g/mol]: 298.81

Physical Properties

Property code	Value	Unit	Source
gf	-164.23	kJ/mol	Joback Method
hf	-541.27	kJ/mol	Joback Method
hfus	39.02	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.431		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	2417.00		NIST Webbook
tb	733.28	K	Joback Method
tc	932.17	K	Joback Method
tf	433.33	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.83	J/mol×K	733.28	Joback Method
cpg	726.56	J/mol×K	899.02	Joback Method
cpg	714.64	J/mol×K	865.88	Joback Method
cpg	701.82	J/mol×K	832.73	Joback Method
cpg	688.09	J/mol×K	799.58	Joback Method
cpg	673.43	J/mol×K	766.43	Joback Method
cpg	737.60	J/mol×K	932.17	Joback Method
dvisc	0.0000846	Pa×s	733.28	Joback Method
dvisc	0.0001082	Pa×s	683.29	Joback Method

dvisc	0.0001438	Pa×s	633.30	Joback Method
dvisc	0.0002006	Pa×s	583.30	Joback Method
dvisc	0.0002978	Pa×s	533.31	Joback Method
dvisc	0.0004800	Pa×s	483.32	Joback Method
dvisc	0.0008637	Pa×s	433.33	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=U360531&Units=SI

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