3-Phenylpropionic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C17H25ClO2/c18-14-8-3-1-2-4-9-15-20-17(19)13-12-16-10-6-5-7-11-16/h5-7,1
InchiKey: MZSRWNOOTLGPIZ-UHFFFAOYSA-N
Formula: C17H25ClO2
SMILES: O=C(CCc1ccccc1)OCCCCCCCCCl
Mol. weight [g/mol]: 296.83

Physical Properties

Property code	Value	Unit	Source
gf	-41.18	kJ/mol	Joback Method
hf	-418.22	kJ/mol	Joback Method
hfus	40.81	kJ/mol	Joback Method
hvap	69.25	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.742		Crippen Method
mcvol	246.310	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	728.76	K	Joback Method
tc	926.10	K	Joback Method
tf	409.85	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.56	J/mol×K	728.76	Joback Method
cpg	758.09	J/mol×K	893.21	Joback Method
cpg	745.41	J/mol×K	860.32	Joback Method
cpg	731.85	J/mol×K	827.43	Joback Method
cpg	717.38	J/mol×K	794.54	Joback Method
cpg	701.96	J/mol×K	761.65	Joback Method
cpg	769.93	J/mol×K	926.10	Joback Method
dvisc	0.0000973	Pa×s	728.76	Joback Method

dvisc	0.0001272	Pa×s	675.61	Joback Method
dvisc	0.0001741	Pa×s	622.46	Joback Method
dvisc	0.0002527	Pa×s	569.30	Joback Method
dvisc	0.0003961	Pa×s	516.15	Joback Method
dvisc	0.0006882	Pa×s	463.00	Joback Method
dvisc	0.0013801	Pa×s	409.85	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=U354744&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