Octanoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H22O2/c1-3-4-5-6-7-11-15(16)17-14-10-8-9-13(2)12-14/h8-10,12H,3-7,11H
InchiKey: VPZWDKNEKVKFOJ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-55.72	kJ/mol	Joback Method
hf	-372.67	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.261		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	650.55	K	Joback Method
tc	848.93	K	Joback Method
tf	369.91	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.11	J/mol×K	650.55	Joback Method
cpg	562.71	J/mol×K	683.61	Joback Method
cpg	578.41	J/mol×K	716.68	Joback Method
cpg	593.23	J/mol×K	749.74	Joback Method
cpg	607.19	J/mol×K	782.80	Joback Method
cpg	620.31	J/mol×K	815.87	Joback Method
cpg	632.62	J/mol×K	848.93	Joback Method
dvisc	0.0015149	Pa×s	369.91	Joback Method

dvisc	0.0008075	Pa×s	416.68	Joback Method
dvisc	0.0004887	Pa×s	463.46	Joback Method
dvisc	0.0003243	Pa×s	510.23	Joback Method
dvisc	0.0002306	Pa×s	557.00	Joback Method
dvisc	0.0001728	Pa×s	603.78	Joback Method
dvisc	0.0001350	Pa×s	650.55	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=U307694&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

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