m-Toluic acid, heptyl ester

Other names: Heptyl 3-methylbenzoate
m-Toluylic acid, heptyl ester
Inchi: InChI=1S/C15H22O2/c1-3-4-5-6-7-11-17-15(16)14-10-8-9-13(2)12-14/h8-10,12H,3-7,11H
InchiKey: FTXBEVYVDATLGN-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCCCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 234.33
CAS: 5462-02-2

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	-4.70		Crippen Method
logp	4.122		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1794.50		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: 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=C5462022&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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