Hexanoic acid, 3-phenylpropyl ester

Other names: 3-phenylpropyl hexanoate
Inchi: InChI=1S/C15H22O2/c1-2-3-5-12-15(16)17-13-8-11-14-9-6-4-7-10-14/h4,6-7,9-10H,2-3,5
InchiKey: RSOGLEKUVSFLMO-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 234.33
CAS: 6281-40-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.09	kJ/mol	Joback Method
hf	-361.20	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.743		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1701.00		NIST Webbook
tb	645.57	K	Joback Method
tc	843.08	K	Joback Method
tf	357.39	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.39	J/mol×K	645.57	Joback Method
cpg	621.23	J/mol×K	810.16	Joback Method
cpg	608.02	J/mol×K	777.24	Joback Method
cpg	593.96	J/mol×K	744.32	Joback Method
cpg	579.02	J/mol×K	711.41	Joback Method
cpg	563.17	J/mol×K	678.49	Joback Method

cpg	633.62	J/mol×K	843.08	Joback Method
dvisc	0.0001364	Pa×s	645.57	Joback Method
dvisc	0.0001776	Pa×s	597.54	Joback Method
dvisc	0.0002424	Pa×s	549.51	Joback Method
dvisc	0.0003510	Pa×s	501.48	Joback Method
dvisc	0.0005498	Pa×s	453.45	Joback Method
dvisc	0.0009578	Pa×s	405.42	Joback Method
dvisc	0.0019370	Pa×s	357.39	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=C6281409&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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