

Hexanoic acid, phenylmethyl ester

Other names:	Benzyl n-hexanoate Benzyl hexanoate Benzyl caproate
Inchi:	InChI=1S/C13H18O2/c1-2-3-5-10-13(14)15-11-12-8-6-4-7-9-12/h4,6-9H,2-3,5,10-11H2,1
InchiKey:	HRSXWUSONDBHSP-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	6938-45-0

Physical Properties

Property code	Value	Unit	Source
gf	-62.93	kJ/mol	Joback Method
hf	-319.92	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.310		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1531.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1506.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1511.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2057.00		NIST Webbook
tb	599.81	K	Joback Method
tc	802.73	K	Joback Method
tf	334.85	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.32	J/molxK	599.81	Joback Method
cpg	459.12	J/molxK	633.63	Joback Method
cpg	474.04	J/molxK	667.45	Joback Method
cpg	488.11	J/molxK	701.27	Joback Method
cpg	501.35	J/molxK	735.09	Joback Method
cpg	513.77	J/molxK	768.91	Joback Method
cpg	525.42	J/molxK	802.73	Joback Method
dvisc	0.0021584	Paxs	334.85	Joback Method
dvisc	0.0011004	Paxs	379.01	Joback Method
dvisc	0.0006457	Paxs	423.17	Joback Method
dvisc	0.0004190	Paxs	467.33	Joback Method
dvisc	0.0002930	Paxs	511.49	Joback Method
dvisc	0.0002169	Paxs	555.65	Joback Method
dvisc	0.0001678	Paxs	599.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6938450&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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