

Benzoic acid, isoheptyl ester

Inchi:	InChI=1S/C13H18O2/c1-11(2)7-6-10-15-13(14)12-8-4-3-5-9-12/h3-5,8-9,11H,6-7,10H2,1
InchiKey:	UUNAMHRNRUJYDO-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CC(C)CCCOC(=O)c1ccccc1
Mol. weight [g/mol]:	206.28

Physical Properties

Property code	Value	Unit	Source
gf	-65.37	kJ/mol	Joback Method
hf	-325.20	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	55.58	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.280		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
tb	599.37	K	Joback Method
tc	806.35	K	Joback Method
tf	319.85	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.71	J/molxK	599.37	Joback Method
cpg	459.89	J/molxK	633.87	Joback Method
cpg	475.13	J/molxK	668.36	Joback Method
cpg	489.48	J/molxK	702.86	Joback Method
cpg	502.95	J/molxK	737.36	Joback Method
cpg	515.57	J/molxK	771.85	Joback Method
cpg	527.37	J/molxK	806.35	Joback Method
dvisc	0.0027865	Paxs	319.85	Joback Method

dvisc	0.0012714	Paxs	366.44	Joback Method
dvisc	0.0006925	Paxs	413.02	Joback Method
dvisc	0.0004266	Paxs	459.61	Joback Method
dvisc	0.0002873	Paxs	506.20	Joback Method
dvisc	0.0002068	Paxs	552.78	Joback Method
dvisc	0.0001567	Paxs	599.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340218&Units=SI
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

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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