

Isovaleric acid, 3-ethylphenyl ester

Inchi:	InChI=1S/C13H18O2/c1-4-11-6-5-7-12(9-11)15-13(14)8-10(2)3/h5-7,9-10H,4,8H2,1-3H3
InchiKey:	DBUQPICDBLXPOV-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCc1cccc(OC(=O)CC(C)C)c1
Mol. weight [g/mol]:	206.28

Physical Properties

Property code	Value	Unit	Source
gf	-75.00	kJ/mol	Joback Method
hf	-336.67	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	56.24	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.200		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinsol	1504.00		NIST Webbook
tb	604.35	K	Joback Method
tc	812.28	K	Joback Method
tf	332.37	K	Joback Method
vc	0.673	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.45	J/molxK	604.35	Joback Method
cpg	459.38	J/molxK	639.01	Joback Method
cpg	474.43	J/molxK	673.66	Joback Method
cpg	488.62	J/molxK	708.32	Joback Method
cpg	501.96	J/molxK	742.97	Joback Method
cpg	514.48	J/molxK	777.63	Joback Method
cpg	526.19	J/molxK	812.28	Joback Method
dvisc	0.0020794	Paxs	332.37	Joback Method
dvisc	0.0010385	Paxs	377.70	Joback Method

dvisc	0.0006019	Paxs	423.03	Joback Method
dvisc	0.0003877	Paxs	468.36	Joback Method
dvisc	0.0002698	Paxs	513.69	Joback Method
dvisc	0.0001992	Paxs	559.02	Joback Method
dvisc	0.0001539	Paxs	604.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360655&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

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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