

4-Ethoxy-3-methylbenzoic acid, ethyl ester

Other names:	Ethyl 4-ethoxy-3-methylbenzoate
Inchi:	InChI=1S/C12H16O3/c1-4-14-11-7-6-10(8-9(11)3)12(13)15-5-2/h6-8H,4-5H2,1-3H3
InchiKey:	GAENXNURLJKMPU-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCOC(=O)c1ccc(OCC)c(C)c1
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-195.61	kJ/mol	Joback Method
hf	-454.44	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.570		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	609.31	K	Joback Method
tc	815.15	K	Joback Method
tf	370.85	K	Joback Method
vc	0.641	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.81	J/mol×K	609.31	Joback Method
cpg	483.69	J/mol×K	780.85	Joback Method
cpg	472.17	J/mol×K	746.54	Joback Method
cpg	459.92	J/mol×K	712.23	Joback Method
cpg	446.94	J/mol×K	677.92	Joback Method
cpg	433.24	J/mol×K	643.62	Joback Method
cpg	494.48	J/mol×K	815.15	Joback Method

dvisc	0.0001427	Paxs	609.31	Joback Method
dvisc	0.0001766	Paxs	569.57	Joback Method
dvisc	0.0002256	Paxs	529.82	Joback Method
dvisc	0.0003000	Paxs	490.08	Joback Method
dvisc	0.0004195	Paxs	450.34	Joback Method
dvisc	0.0006260	Paxs	410.59	Joback Method
dvisc	0.0010176	Paxs	370.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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