

Ethyl-2,4,6-trimethylbenzoate

Other names:	Benzoic acid, 2,4,6-trimethyl-, ethyl ester
Inchi:	InChI=1S/C12H16O2/c1-5-14-12(13)11-9(3)6-8(2)7-10(11)4/h6-7H,5H2,1-4H3
InchiKey:	ZXTXIZPSMQCYBN-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCOC(=O)c1c(C)cc(C)cc1C
Mol. weight [g/mol]:	192.25
CAS:	1754-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-100.24	kJ/mol	Joback Method
hf	-333.69	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	55.72	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.789		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
tb	591.87	K	Joback Method
tc	800.82	K	Joback Method
tf	361.14	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.00	J/molxK	591.87	Joback Method
cpg	407.43	J/molxK	626.70	Joback Method
cpg	421.16	J/molxK	661.52	Joback Method
cpg	434.17	J/molxK	696.35	Joback Method
cpg	446.48	J/molxK	731.17	Joback Method
cpg	458.09	J/molxK	766.00	Joback Method
cpg	469.00	J/molxK	800.82	Joback Method
dvisc	0.0010751	Paxs	361.14	Joback Method

dvisc	0.0006856	Paxs	399.60	Joback Method
dvisc	0.0004732	Paxs	438.05	Joback Method
dvisc	0.0003467	Paxs	476.50	Joback Method
dvisc	0.0002661	Paxs	514.96	Joback Method
dvisc	0.0002119	Paxs	553.41	Joback Method
dvisc	0.0001738	Paxs	591.87	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=C1754558&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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