

Ethyl 4-t-butylbenzoate

Other names:	Ethyl 4-tert-butylbenzoate Benzoic acid, 4-(1,1-dimethylethyl)-, ethyl ester ethyl 4-(1,1-dimethylethyl)benzoate
Inchi:	InChI=1S/C13H18O2/c1-5-15-12(14)10-6-8-11(9-7-10)13(2,3)4/h6-9H,5H2,1-4H3
InchiKey:	LIQWHXBLFOERRD-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCOC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	206.28
CAS:	5406-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-69.72	kJ/mol	Joback Method
hf	-340.14	kJ/mol	Joback Method
hfus	18.45	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.161		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	601.56	K	Joback Method
tc	817.36	K	Joback Method
tf	349.79	K	Joback Method
vc	0.668	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.22	J/mol×K	601.56	Joback Method
cpg	462.62	J/mol×K	637.53	Joback Method
cpg	477.98	J/mol×K	673.49	Joback Method
cpg	492.35	J/mol×K	709.46	Joback Method

cpg	505.78	J/molxK	745.43	Joback Method
cpg	518.30	J/molxK	781.39	Joback Method
cpg	529.96	J/molxK	817.36	Joback Method
dvisc	0.0018655	Paxs	349.79	Joback Method
dvisc	0.0009730	Paxs	391.75	Joback Method
dvisc	0.0005756	Paxs	433.71	Joback Method
dvisc	0.0003736	Paxs	475.67	Joback Method
dvisc	0.0002601	Paxs	517.64	Joback Method
dvisc	0.0001911	Paxs	559.60	Joback Method
dvisc	0.0001467	Paxs	601.56	Joback Method

Sources

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=C5406575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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