3'-ETHYLACETOPHENONE

Other names: 1-(3-Ethylphenyl)ethanone
3'-Ethylacetophenone
3-Ethylacetophenone
Inchi: InChI=1S/C10H12O/c1-3-9-5-4-6-10(7-9)8(2)11/h4-7H,3H2,1-2H3
InchiKey: ZRYRILAFFDKOPB-UHFFFAOYSA-N
Formula: C10H12O
SMILES: CCc1cccc(C(C)=O)c1
Mol. weight [g/mol]: 148.21

Physical Properties

Property code	Value	Unit	Source
af	0.4679		Cheméo Relay (1.0)
gf	7.18	kJ/mol	Joback Method
hf	-159.29	kJ/mol	Cheméo Relay (1.0)
hfus	16.91	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
log10ws	-2.69		Cheméo Relay (1.0)
logp	2.452		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1186.00		NIST Webbook
rinpol	1210.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
tb	506.28	K	Cheméo Relay (1.0)
tc	716.36	K	Cheméo Relay (1.0)
tf	257.57	K	Cheméo Relay (1.0)
vc	0.479	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.66	J/mol×K	513.73	Joback Method

cpg	346.84	J/mol×K	729.82	Joback Method
cpg	336.91	J/mol×K	693.81	Joback Method
cpg	326.32	J/mol×K	657.79	Joback Method
cpg	315.02	J/mol×K	621.78	Joback Method
cpg	303.00	J/mol×K	585.76	Joback Method
cpg	290.22	J/mol×K	549.75	Joback Method
dvisc	0.0005549	Pa×s	402.53	Joback Method
dvisc	0.0002503	Pa×s	513.73	Joback Method
dvisc	0.0003132	Pa×s	476.66	Joback Method
dvisc	0.0004070	Pa×s	439.60	Joback Method
dvisc	0.0022588	Pa×s	291.33	Joback Method
dvisc	0.0008058	Pa×s	365.46	Joback Method
dvisc	0.0012729	Pa×s	328.40	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22699703&Units=SI

Legend

af: Acentric Factor
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
ie: Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume