Ethylbenzene-d10

Other names: Benzene-d5-, ethyl-d5-
(2H10)ethylbenzene
Inchi: InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h3-7H,2H2,1H3/i1D3,2D2,3D,4D,5D,6D,7D
InchiKey: YNQLUTRBYVCPMQ-CFTAVCBPSA-N
Formula: C8D10
SMILES: CCc1ccccc1
Mol. weight [g/mol]: 116.23
CAS: 25837-05-2

Physical Properties

Property code	Value	Unit	Source
gf	128.89	kJ/mol	Joback Method
hf	28.08	kJ/mol	Joback Method
hfus	10.52	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.249		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
rinpol	852.00		NIST Webbook
ripol	1105.00		NIST Webbook
ripol	1124.00		NIST Webbook
ripol	1105.00		NIST Webbook
tb	409.12	K	Joback Method
tc	618.55	K	Joback Method
tf	206.34	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.34	J/mol×K	409.12	Joback Method
cpg	232.46	J/mol×K	583.65	Joback Method
cpg	222.37	J/mol×K	548.74	Joback Method

cpg	211.64	J/mol×K	513.84	Joback Method
cpg	200.25	J/mol×K	478.93	Joback Method
cpg	188.16	J/mol×K	444.03	Joback Method
cpg	241.94	J/mol×K	618.55	Joback Method
dvisc	0.0002314	Pa×s	409.12	Joback Method
dvisc	0.0002946	Pa×s	375.32	Joback Method
dvisc	0.0003935	Pa×s	341.53	Joback Method
dvisc	0.0005599	Pa×s	307.73	Joback Method
dvisc	0.0008693	Pa×s	273.93	Joback Method
dvisc	0.0015274	Pa×s	240.14	Joback Method
dvisc	0.0032282	Pa×s	206.34	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=C25837052&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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