

«alpha», «beta»-Dimethylstyrene

Other names:	Benzene, (1-methyl-1-propenyl)- (1-methylpropenyl)benzene
Inchi:	InChI=1S/C10H12/c1-3-9(2)10-7-5-4-6-8-10/h3-8H,1-2H3
InchiKey:	UGUYQBMBIJFNRM-UHFFFAOYSA-N
Formula:	C10H12
SMILES:	CC=C(C)c1ccccc1
Mol. weight [g/mol]:	132.20
CAS:	2082-61-3

Physical Properties

Property code	Value	Unit	Source
gf	217.40	kJ/mol	Joback Method
hf	94.23	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	40.17	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.110		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1090.70		NIST Webbook
rinpol	1090.70		NIST Webbook
rinpol	1090.70		NIST Webbook
tb	461.65 ± 6.00	K	NIST Webbook
tb	463.15 ± 5.00	K	NIST Webbook
tb	465.15 ± 5.00	K	NIST Webbook
tb	463.00 ± 5.00	K	NIST Webbook
tb	461.15 ± 6.00	K	NIST Webbook
tb	457.15 ± 5.00	K	NIST Webbook
tc	678.24	K	Joback Method
tf	209.84	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.06	J/mol×K	458.92	Joback Method
cpg	255.09	J/mol×K	495.47	Joback Method
cpg	269.14	J/mol×K	532.03	Joback Method
cpg	282.26	J/mol×K	568.58	Joback Method
cpg	294.51	J/mol×K	605.14	Joback Method
cpg	305.95	J/mol×K	641.69	Joback Method
cpg	316.62	J/mol×K	678.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2082613&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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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