

4-Vinyl-.alpha.-methylstyrene

Other names:	1-Vinyl-4«alpha»-methylstyrene
Inchi:	InChI=1S/C11H12/c1-4-10-5-7-11(8-6-10)9(2)3/h4-8H,1-2H2,3H3
InchiKey:	NRPJKIBPPQLLDX-UHFFFAOYSA-N
Formula:	C11H12
SMILES:	C=Cc1ccc(C(=C)C)cc1
Mol. weight [g/mol]:	144.22

Physical Properties

Property code	Value	Unit	Source
af	0.4048		Cheméo Relay (1.0)
hf	174.09	kJ/mol	Cheméo Relay (1.0)
hfus	14.03	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-3.95		Cheméo Relay (1.0)
logp	3.363		Crippen Method
mcvol	133.490	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1218.50		NIST Webbook
rinpol	1218.50		NIST Webbook
tb	490.86	K	Cheméo Relay (1.0)
tc	701.91	K	Cheméo Relay (1.0)
tf	276.55	K	Cheméo Relay (1.0)
vc	0.488	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.83	J/mol×K	475.98	Joback Method
cpg	280.46	J/mol×K	512.06	Joback Method
cpg	294.18	J/mol×K	548.15	Joback Method
cpg	307.06	J/mol×K	584.23	Joback Method
cpg	319.12	J/mol×K	620.32	Joback Method
cpg	330.41	J/mol×K	656.40	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R11410&Units=SI>

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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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