1,3,5-Cycloheptatriene, 3,7,7-trimethyl-

Other names:	3,7,7-Trimethylcyclohepta-1,3,5-triene
	3,7,7-Trimethyl-1,3,5-cycloheptatriene
Inchi:	InChI=1S/C10H14/c1-9-5-4-7-10(2,3)8-6-9/h4-8H,1-3H3
InchiKey:	VOURXYUVXXLJMD-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	CC1=CC=CC(C)(C)C=C1
Mol. weight [g/mol]:	134.22
CAS:	3479-89-8

Physical Properties

Property code	Value	Unit	Source
gf	120.43	kJ/mol	Joback Method
hf	-24.46	kJ/mol	Joback Method
hfus	8.37	kJ/mol	Joback Method
hvap	38.84	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.085		Crippen Method
mcvol	128.000	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	972.60		NIST Webbook
rinpol	953.00		NIST Webbook
tb	454.72	K	Joback Method
tc	676.79	K	Joback Method
tf	245.02	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.90	J/mol×K	454.72	Joback Method
cpg	273.63	J/mol×K	491.73	Joback Method

cpg	289.18	J/mol×K	528.74	Joback Method
cpg	303.65	J/mol×K	565.76	Joback Method
cpg	317.18	J/mol×K	602.77	Joback Method
cpg	329.86	J/mol×K	639.78	Joback Method
cpg	341.81	J/mol×K	676.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3479898&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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