Octalene

Inchi:	InChI=1S/C14H12/c1-2-6-10-14-12-8-4-3-7-11-13(14)9-5-1/h1-12H/b2-1-,4-3-,5-1-,6-2-,7
InchiKey:	OVPVGJFDFSJUIG-VFLSUHNHSA-N
Formula:	C14H12
SMILES:	c1cccc2ccccccc-2cc1
Mol. weight [g/mol]:	180.25
CAS:	257-55-6

Physical Properties

Property code	Value	Unit	Source
gf	297.58	kJ/mol	Joback Method
hf	551.50	kJ/mol	NIST Webbook
hfus	17.12	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.916		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	580.78	K	Joback Method
tc	841.19	K	Joback Method
tf	294.10	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.44	J/mol×K	580.78	Joback Method
cpg	432.53	J/mol×K	797.79	Joback Method
cpg	419.72	J/mol×K	754.39	Joback Method
cpg	405.58	J/mol×K	710.99	Joback Method
cpg	390.04	J/mol×K	667.58	Joback Method
cpg	373.01	J/mol×K	624.18	Joback Method
cpg	444.08	J/mol×K	841.19	Joback Method
dvisc	0.0001096	Pa×s	580.78	Joback Method
dvisc	0.0001499	Pa×s	533.00	Joback Method

dvisc	0.0002180	Pa×s	485.22	Joback Method
dvisc	0.0003439	Pa×s	437.44	Joback Method
dvisc	0.0006070	Pa×s	389.66	Joback Method
dvisc	0.0012556	Pa×s	341.88	Joback Method
dvisc	0.0032891	Pa×s	294.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C257556&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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