4,7-Dimethyl-1-tetralone

Other names: 4,7-Dimethyltetral-1-one
Inchi: InChI=1S/C12H14O/c1-8-3-5-10-9(2)4-6-12(13)11(10)7-8/h3,5,7,9H,4,6H2,1-2H3
InchiKey: SQESYXTWWGWCFK-UHFFFAOYSA-N
Formula: C12H14O
SMILES: Cc1ccc2c(c1)C(=O)CCC2C
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	69.37	kJ/mol	Joback Method
hf	-148.48	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.075		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1509.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	589.43	K	Joback Method
tc	829.72	K	Joback Method
tf	359.10	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.04	J/mol×K	589.43	Joback Method
cpg	381.43	J/mol×K	629.48	Joback Method
cpg	397.74	J/mol×K	669.53	Joback Method

cpg	413.00	J/mol×K	709.57	Joback Method
cpg	427.23	J/mol×K	749.62	Joback Method
cpg	440.46	J/mol×K	789.67	Joback Method
cpg	452.72	J/mol×K	829.72	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=R228838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume