(3a«alpha»,4«alpha»,7«alpha»,7a«alpha»)-3a,4,7,7

Inchi: InChI=1S/C10H12/c1-2-9-7-4-5-8(6-7)10(9)3-1/h1-2,4-5,7-10H,3,6H2/t7-,8-,9-,10+/m1/s1
InchiKey: HECLRDQVFMWTQS-KYXWUPHJSA-N
Formula: C10H12
SMILES: C1=CC2C3C=CC(C3)C2C1
Mol. weight [g/mol]: 132.20
CAS: 1755-01-7

Physical Properties

Property code	Value	Unit	Source
chs	-5766.80 ± 5.90	kJ/mol	NIST Webbook
gf	255.68	kJ/mol	Joback Method
hf	57.73	kJ/mol	Joback Method
hfus	17.48	kJ/mol	Joback Method
hvap	38.04	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.385		Crippen Method
mcvol	110.580	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
ss	230.00	J/mol×K	NIST Webbook
tb	446.34	K	Joback Method
tc	664.47	K	Joback Method
tf	250.04	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.43	J/mol×K	628.12	Joback Method
cpg	308.96	J/mol×K	591.76	Joback Method
cpg	294.37	J/mol×K	555.41	Joback Method
cpg	278.56	J/mol×K	519.05	Joback Method
cpg	261.44	J/mol×K	482.70	Joback Method
cpg	242.89	J/mol×K	446.34	Joback Method
cpg	334.89	J/mol×K	664.47	Joback Method

cps	188.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0004087	Pa×s	250.04	Joback Method
dvisc	0.0010224	Pa×s	446.34	Joback Method
dvisc	0.0009322	Pa×s	413.62	Joback Method
dvisc	0.0008365	Pa×s	380.91	Joback Method
dvisc	0.0007356	Pa×s	348.19	Joback Method
dvisc	0.0006298	Pa×s	315.47	Joback Method
dvisc	0.0005202	Pa×s	282.76	Joback Method
hfust	2.22	kJ/mol	304.80	NIST Webbook
hfust	1.79	kJ/mol	304.70	NIST Webbook
hvapt	43.60	kJ/mol	398.00	NIST Webbook

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=C1755017&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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