trans-(2,3,3a,7a-Tetrahydro-1H-indene-4-carbalde

Inchi: InChI=1S/C10H12O/c11-7-9-5-1-3-8-4-2-6-10(8)9/h1,3,5,7-8,10H,2,4,6H2/t8-,10-/m0/s1
InchiKey: NRPGDWVRKOJMEE-WPRPVWTQSA-N
Formula: C10H12O
SMILES: O=CC1=CC=CC2CCCC12
Mol. weight [g/mol]: 148.20

Physical Properties

Property code	Value	Unit	Source
gf	69.29	kJ/mol	Joback Method
hf	-104.10	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.098		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1254.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	506.45	K	Joback Method
tc	730.39	K	Joback Method
tf	283.82	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.32	J/mol×K	506.45	Joback Method
cpg	297.58	J/mol×K	543.77	Joback Method
cpg	312.72	J/mol×K	581.10	Joback Method
cpg	326.82	J/mol×K	618.42	Joback Method
cpg	339.93	J/mol×K	655.74	Joback Method
cpg	352.11	J/mol×K	693.07	Joback Method

cpg	363.43	J/mol×K	730.39	Joback Method
dvisc	0.0021391	Pa×s	283.82	Joback Method
dvisc	0.0015377	Pa×s	320.93	Joback Method
dvisc	0.0011837	Pa×s	358.03	Joback Method
dvisc	0.0009570	Pa×s	395.13	Joback Method
dvisc	0.0008026	Pa×s	432.24	Joback Method
dvisc	0.0006920	Pa×s	469.34	Joback Method
dvisc	0.0006098	Pa×s	506.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586753&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

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
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