Methyl trans-2,3,3a,7a-tetrahydro-1H-indene-4-carboxylat

Inchi: InChI=1S/C11H14O2/c1-13-11(12)10-7-3-5-8-4-2-6-9(8)10/h3,5,7-9H,2,4,6H2,1H3/t8-,9+

InchiKey: ABRJMTSLLBQAHF-DTWKUNHWSA-N

Formula: C11H14O2

SMILES: COC(=O)C1=CC=CC2CCCC12

Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-56.69	kJ/mol	Joback Method
hf	-283.96	kJ/mol	Joback Method
hfus	19.06	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.072		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1368.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	556.96	K	Joback Method
tc	779.82	K	Joback Method
tf	325.25	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.51	J/mol×K	556.96	Joback Method
cpg	369.38	J/mol×K	594.10	Joback Method
cpg	385.17	J/mol×K	631.25	Joback Method
cpg	399.93	J/mol×K	668.39	Joback Method
cpg	413.72	J/mol×K	705.53	Joback Method
cpg	426.56	J/mol×K	742.68	Joback Method
cpg	438.51	J/mol×K	779.82	Joback Method
dvisc	0.0019518	Pa×s	325.25	Joback Method

dvisc	0.0013720	Pa×s	363.87	Joback Method
dvisc	0.0010320	Pa×s	402.49	Joback Method
dvisc	0.0008159	Pa×s	441.11	Joback Method
dvisc	0.0006699	Pa×s	479.72	Joback Method
dvisc	0.0005665	Pa×s	518.34	Joback Method
dvisc	0.0004903	Pa×s	556.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586748&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
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