Ethyl 3-(chlorocarbonyl)bicyclo[2.2.1]hept-5-ene-2-carb

Inchi: InChI=1S/C11H13ClO3/c1-2-15-11(14)9-7-4-3-6(5-7)8(9)10(12)13/h3-4,6-9H,2,5H2,1H3

InchiKey: UFJRFJAUWQRPBW-UHFFFAOYSA-N

Formula: C11H13ClO3

SMILES: CCOC(=O)C1C2C=CC(C2)C1C(=O)Cl

Mol. weight [g/mol]: 228.67

Physical Properties

Property code	Value	Unit	Source
gf	-209.09	kJ/mol	Joback Method
hf	-486.95	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	60.04	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.753		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
tb	626.24	K	Joback Method
tc	842.44	K	Joback Method
tf	390.38	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.30	J/mol×K	626.24	Joback Method
cpg	486.97	J/mol×K	806.41	Joback Method
cpg	475.79	J/mol×K	770.37	Joback Method
cpg	463.78	J/mol×K	734.34	Joback Method
cpg	450.90	J/mol×K	698.31	Joback Method
cpg	437.08	J/mol×K	662.27	Joback Method
cpg	497.38	J/mol×K	842.44	Joback Method
dvisc	0.0013176	Pa×s	626.24	Joback Method

dvisc	0.0014235	Pa×s	586.93	Joback Method
dvisc	0.0015550	Pa×s	547.62	Joback Method
dvisc	0.0017220	Pa×s	508.31	Joback Method
dvisc	0.0019399	Pa×s	469.00	Joback Method
dvisc	0.0022336	Pa×s	429.69	Joback Method
dvisc	0.0026457	Pa×s	390.38	Joback Method

Sources

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=U375830&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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