Cycloheptanecarboxylic acid

Inchi: InChI=1S/C8H14O2/c9-8(10)7-5-3-1-2-4-6-7/h7H,1-6H2,(H,9,10)
InchiKey: VZFUCHSFHOYXIS-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: O=C(O)C1CCCCCC1
Mol. weight [g/mol]: 142.20
CAS: 1460-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-236.91	kJ/mol	Joback Method
hf	-425.10	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.041		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	552.31	K	Joback Method
tc	758.79	K	Joback Method
tf	294.53	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.08	J/mol×K	552.31	Joback Method
cpg	310.66	J/mol×K	586.72	Joback Method
cpg	324.43	J/mol×K	621.14	Joback Method
cpg	337.40	J/mol×K	655.55	Joback Method
cpg	349.58	J/mol×K	689.96	Joback Method
cpg	360.99	J/mol×K	724.38	Joback Method
cpg	371.66	J/mol×K	758.79	Joback Method
dvisc	0.0233646	Pa×s	294.53	Joback Method
dvisc	0.0054515	Pa×s	337.49	Joback Method

dvisc	0.0017669	Pa×s	380.46	Joback Method
dvisc	0.0007198	Pa×s	423.42	Joback Method
dvisc	0.0003460	Pa×s	466.38	Joback Method
dvisc	0.0001882	Pa×s	509.35	Joback Method
dvisc	0.0001125	Pa×s	552.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	409.70	K	1.00	NIST Webbook
tbrp	529.20	K	94.80	NIST Webbook
tbrp	403.70	K	1.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460168&Units=SI

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

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