

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)C1CCCCC1
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
hf	-501.02	kJ/mol	Cheméo Relay (1.0)
hfus	11.90	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Cheméo Relay (1.0)
ie	10.09	eV	Cheméo Relay (1.0)
log10ws	-1.77		Cheméo Relay (1.0)
logp	2.041		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
tb	521.47	K	Cheméo Relay (1.0)
tf	330.42	K	Cheméo Relay (1.0)

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

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460168&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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