2-Propyltetrahydropyran

Inchi: InChI=1S/C8H16O/c1-2-5-8-6-3-4-7-9-8/h8H,2-7H2,1H3
InchiKey: YHQBBDKFBJYMPJ-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC1CCCCO1
Mol. weight [g/mol]: 128.21
CAS: 3857-17-8

Physical Properties

Property code	Value	Unit	Source
gf	-45.19	kJ/mol	Joback Method
hf	-286.13	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	38.34	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.356		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	958.00		NIST Webbook
tb	428.94	K	Joback Method
tc	629.92	K	Joback Method
tf	213.87	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.71	J/mol×K	428.94	Joback Method
cpg	321.73	J/mol×K	596.43	Joback Method
cpg	307.87	J/mol×K	562.93	Joback Method
cpg	293.25	J/mol×K	529.43	Joback Method
cpg	277.87	J/mol×K	495.93	Joback Method
cpg	261.70	J/mol×K	462.44	Joback Method

cpg	334.85	J/mol×K	629.92	Joback Method
dvisc	0.0003157	Pa×s	428.94	Joback Method
dvisc	0.0004265	Pa×s	393.10	Joback Method
dvisc	0.0006119	Pa×s	357.25	Joback Method
dvisc	0.0009518	Pa×s	321.40	Joback Method
dvisc	0.0016539	Pa×s	285.56	Joback Method
dvisc	0.0033681	Pa×s	249.72	Joback Method
dvisc	0.0087057	Pa×s	213.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3857178&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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