2-methyl-(E)-2-pentenal

Other names: (E)-2-Methylpent-2-enal
trans-2-methyl-2-penten-1-al
(E)-2-methyl-2-pentenal
Inchi: InChI=1S/C6H10O/c1-3-4-6(2)5-7/h4-5H,3H2,1-2H3/b6-4+
InchiKey: IDEYZABHVQLHAF-GQCTYLIASA-N
Formula: C6H10O
SMILES: CCC=C(C)C=O
Mol. weight [g/mol]: 98.14
CAS: 14250-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-28.21	kJ/mol	Joback Method
hf	-145.32	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	831.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	820.00		NIST Webbook
ripol	1175.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1176.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1176.00		NIST Webbook
ripol	1176.00		NIST Webbook
tb	389.38	K	Joback Method
tc	574.52	K	Joback Method
tf	180.34	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.68	J/mol×K	389.38	Joback Method
cpg	174.31	J/mol×K	420.24	Joback Method
cpg	183.47	J/mol×K	451.09	Joback Method
cpg	192.18	J/mol×K	481.95	Joback Method
cpg	200.45	J/mol×K	512.80	Joback Method
cpg	208.31	J/mol×K	543.66	Joback Method
cpg	215.78	J/mol×K	574.52	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=C14250965&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
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