

methyl 3-methyl-3-pentenoate

Inchi:	InChI=1S/C7H12O2/c1-4-6(2)5-7(8)9-3/h4H,5H2,1-3H3/b6-4+
InchiKey:	OUARJKDCCMXOEF-GQCTYLIASA-N
Formula:	C7H12O2
SMILES:	CC=C(C)CC(=O)OC
Mol. weight [g/mol]:	128.17
CAS:	2258-58-4

Physical Properties

Property code	Value	Unit	Source
gf	-154.19	kJ/mol	Joback Method
hf	-325.18	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
ripol	1211.00		NIST Webbook
ripol	1246.00		NIST Webbook
ripol	1211.00		NIST Webbook
tb	439.89	K	Joback Method
tc	628.49	K	Joback Method
tf	221.77	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.62	J/molxK	439.89	Joback Method
cpg	233.55	J/molxK	471.32	Joback Method
cpg	244.02	J/molxK	502.76	Joback Method
cpg	254.05	J/molxK	534.19	Joback Method
cpg	263.64	J/molxK	565.63	Joback Method
cpg	272.80	J/molxK	597.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.89075e+01
Coeff. B	-5.07474e+03
Coeff. C	-6.56080e+01
Temperature range (K), min.	338.15
Temperature range (K), max.	438.86

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334988&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
riPOL:	Polar retention indices

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

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