

2-Propenoic acid, pentyl ester

Other names:	2-Propenoic acid,n-pentyl ester Pentyl acrylate acrylic acid, pentyl ester amyl acrylate n-Amyl acrylate n-pentyl acrylate pentyl 2-propenoate
Inchi:	InChI=1S/C8H14O2/c1-3-5-6-7-10-8(9)4-2/h4H,2-3,5-7H2,1H3
InchiKey:	ULDDEWDFUNBUKM-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	C=CC(=O)OCCCC
Mol. weight [g/mol]:	142.20
CAS:	2998-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-129.60	kJ/mol	Joback Method
hf	-327.82	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mvol	126.720	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	973.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1273.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1273.00		NIST Webbook

tb	455.41	K	Joback Method
tc	633.98	K	Joback Method
tf	250.32	K	Joback Method
vc	0.488	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.07	J/mol×K	455.41	Joback Method
cpg	274.71	J/mol×K	485.17	Joback Method
cpg	285.90	J/mol×K	514.93	Joback Method
cpg	296.66	J/mol×K	544.69	Joback Method
cpg	306.99	J/mol×K	574.46	Joback Method
cpg	316.89	J/mol×K	604.22	Joback Method
cpg	326.37	J/mol×K	633.98	Joback Method
dvisc	0.0029783	Paxs	250.32	Joback Method
dvisc	0.0015454	Paxs	284.50	Joback Method
dvisc	0.0009231	Paxs	318.68	Joback Method
dvisc	0.0006093	Paxs	352.87	Joback Method
dvisc	0.0004328	Paxs	387.05	Joback Method
dvisc	0.0003249	Paxs	421.23	Joback Method
dvisc	0.0002547	Paxs	455.41	Joback Method
hvapt	44.90	kJ/mol	382.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2998234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
High-Pressure Phase Behavior for Pentyl Acrylate and Pentyl Methacrylate	https://www.doi.org/10.1021/je060122s
Joback Method: Supercritical Carbon Dioxide	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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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