

Valeric acid, 3-methylphenyl ester

Inchi:	InChI=1S/C12H16O2/c1-3-4-8-12(13)14-11-7-5-6-10(2)9-11/h5-7,9H,3-4,8H2,1-2H3
InchiKey:	MEKODTPFXNDIKN-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	192.25

Physical Properties

Property code	Value	Unit	Source
gf	-80.98	kJ/mol	Joback Method
hf	-310.75	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.091		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinsol	1432.00		NIST Webbook
tb	581.91	K	Joback Method
tc	788.90	K	Joback Method
tf	336.10	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.77	J/molxK	581.91	Joback Method
cpg	408.69	J/molxK	616.41	Joback Method
cpg	422.81	J/molxK	650.91	Joback Method
cpg	436.14	J/molxK	685.41	Joback Method
cpg	448.71	J/molxK	719.90	Joback Method
cpg	460.52	J/molxK	754.40	Joback Method
cpg	471.60	J/molxK	788.90	Joback Method
dvisc	0.0017122	Paxs	336.10	Joback Method
dvisc	0.0009597	Paxs	377.07	Joback Method

dvisc	0.0006026	Paxs	418.04	Joback Method
dvisc	0.0004111	Paxs	459.00	Joback Method
dvisc	0.0002986	Paxs	499.97	Joback Method
dvisc	0.0002277	Paxs	540.94	Joback Method
dvisc	0.0001803	Paxs	581.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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