

2-Methylpentanoic acid, 2-biphenyl ester

Inchi:	InChI=1S/C18H20O2/c1-3-9-14(2)18(19)20-17-13-8-7-12-16(17)15-10-5-4-6-11-15/h4-8,
InchiKey:	BHZVELAKMDGMRN-UHFFFAOYSA-N
Formula:	C18H20O2
SMILES:	CCCC(C)C(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	268.35

Physical Properties

Property code	Value	Unit	Source
gf	79.51	kJ/mol	Joback Method
hf	-203.34	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.695		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1954.00		NIST Webbook
tb	745.43	K	Joback Method
tc	974.99	K	Joback Method
tf	415.14	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.40	J/molxK	745.43	Joback Method
cpg	698.31	J/molxK	936.73	Joback Method
cpg	686.27	J/molxK	898.47	Joback Method
cpg	673.11	J/molxK	860.21	Joback Method
cpg	658.78	J/molxK	821.95	Joback Method
cpg	643.23	J/molxK	783.69	Joback Method
cpg	709.30	J/molxK	974.99	Joback Method
dvisc	0.0000895	Paxs	745.43	Joback Method
dvisc	0.0001161	Paxs	690.38	Joback Method

dvisc	0.0001574	Paxs	635.33	Joback Method
dvisc	0.0002262	Paxs	580.28	Joback Method
dvisc	0.0003506	Paxs	525.24	Joback Method
dvisc	0.0006022	Paxs	470.19	Joback Method
dvisc	0.0011940	Paxs	415.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357385&Units=SI

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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