

2-Methylvaleric acid, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C19H22O3/c1-3-7-15(2)19(20)22-18-12-10-17(11-13-18)21-14-16-8-5-4-6-9-10
InchiKey:	QRXHTIGWKVQUAF-UHFFFAOYSA-N
Formula:	C19H22O3
SMILES:	CCCC(C)C(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	298.38

Physical Properties

Property code	Value	Unit	Source
gf	-17.07	kJ/mol	Joback Method
hf	-356.20	kJ/mol	Joback Method
hfus	33.11	kJ/mol	Joback Method
hvap	74.28	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.607		Crippen Method
mvol	244.360	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	790.73	K	Joback Method
tc	1014.28	K	Joback Method
tf	448.64	K	Joback Method
vc	0.919	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.10	J/molxK	790.73	Joback Method
cpg	726.50	J/molxK	827.99	Joback Method
cpg	741.60	J/molxK	865.25	Joback Method
cpg	755.44	J/molxK	902.51	Joback Method
cpg	768.08	J/molxK	939.76	Joback Method
cpg	779.53	J/molxK	977.02	Joback Method
cpg	789.84	J/molxK	1014.28	Joback Method
dvisc	0.0007740	Paxs	448.64	Joback Method

dvisc	0.0003983	Paxs	505.66	Joback Method
dvisc	0.0002345	Paxs	562.67	Joback Method
dvisc	0.0001522	Paxs	619.69	Joback Method
dvisc	0.0001063	Paxs	676.70	Joback Method
dvisc	0.0000784	Paxs	733.72	Joback Method
dvisc	0.0000605	Paxs	790.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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