

Octanoic acid, 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C21H26O3/c1-2-3-4-5-9-12-21(22)24-20-15-13-19(14-16-20)23-17-18-10-7-6-8
InchiKey:	SATIMNZTDGRRFK-UHFFFAOYSA-N
Formula:	C21H26O3
SMILES:	CCCCCCCC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	326.43

Physical Properties

Property code	Value	Unit	Source
gf	2.21	kJ/mol	Joback Method
hf	-392.20	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	79.12	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.532		Crippen Method
mvol	272.540	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	836.93	K	Joback Method
tc	1052.79	K	Joback Method
tf	486.18	K	Joback Method
vc	1.038	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.44	J/molxK	836.93	Joback Method
cpg	840.79	J/molxK	872.91	Joback Method
cpg	855.87	J/molxK	908.88	Joback Method
cpg	869.73	J/molxK	944.86	Joback Method
cpg	882.39	J/molxK	980.84	Joback Method
cpg	893.91	J/molxK	1016.82	Joback Method
cpg	904.32	J/molxK	1052.79	Joback Method
dvisc	0.0005623	Paxs	486.18	Joback Method

dvisc	0.0003035	Paxs	544.64	Joback Method
dvisc	0.0001846	Paxs	603.10	Joback Method
dvisc	0.0001226	Paxs	661.55	Joback Method
dvisc	0.0000870	Paxs	720.01	Joback Method
dvisc	0.0000650	Paxs	778.47	Joback Method
dvisc	0.0000506	Paxs	836.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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