2-[2'-(Alpha-methylbenzyloxy)ethoxy]ethyl benzoate

Inchi: InChI=1S/C19H22O4/c1-16(17-8-4-2-5-9-17)22-14-12-21-13-15-23-19(20)18-10-6-3-7-11

InchiKey: NSSPMFHHOOGMCN-UHFFFAOYSA-N

Formula: C19H22O4

SMILES: CC(OCCOCCOC(=O)c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 314.38

CAS: 116495-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-112.44	kJ/mol	Joback Method
hf	-476.95	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	76.03	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.638		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
tb	808.17	K	Joback Method
tc	1029.08	K	Joback Method
tf	458.35	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.06	J/mol×K	808.17	Joback Method
cpg	754.95	J/mol×K	844.99	Joback Method
cpg	769.50	J/mol×K	881.81	Joback Method
cpg	782.76	J/mol×K	918.62	Joback Method
cpg	794.73	J/mol×K	955.44	Joback Method
cpg	805.46	J/mol×K	992.26	Joback Method
cpg	814.97	J/mol×K	1029.08	Joback Method
dvisc	0.0006501	Pa×s	458.35	Joback Method
dvisc	0.0003250	Pa×s	516.65	Joback Method

dvisc	0.0001870	Pa×s	574.96	Joback Method
dvisc	0.0001191	Pa×s	633.26	Joback Method
dvisc	0.0000819	Pa×s	691.56	Joback Method
dvisc	0.0000596	Pa×s	749.87	Joback Method
dvisc	0.0000455	Pa×s	808.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495717&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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