

1,2-Benzenedicarboxylic acid, bis(ethoxyethoxyethyl) ester

Other names:	bis(2-(2-ethoxyethoxy)ethyl) phthalate
Inchi:	InChI=1S/C20H30O8/c1-3-23-9-11-25-13-15-27-19(21)17-7-5-6-8-18(17)20(22)28-16-14
InchiKey:	BWTZODIETZQWSD-UHFFFAOYSA-N
Formula:	C20H30O8
SMILES:	CCOCCOCCOC(=O)c1ccccc1C(=O)OCCOCCOCC
Mol. weight [g/mol]:	398.45
CAS:	117-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-667.54	kJ/mol	Joback Method
hf	-1249.55	kJ/mol	Joback Method
hfus	51.53	kJ/mol	Joback Method
hvap	91.00	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.106		Crippen Method
mcvol	307.260	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
tb	930.92	K	Joback Method
tc	1140.73	K	Joback Method
tf	587.34	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.16	J/mol×K	930.92	Joback Method
cpg	1044.88	J/mol×K	1105.76	Joback Method
cpg	1037.94	J/mol×K	1070.80	Joback Method
cpg	1029.27	J/mol×K	1035.83	Joback Method
cpg	1018.90	J/mol×K	1000.86	Joback Method
cpg	1006.85	J/mol×K	965.89	Joback Method
cpg	1050.05	J/mol×K	1140.73	Joback Method
dvisc	0.0000169	Pa×s	930.92	Joback Method

dvisc	0.0000214	Pa×s	873.66	Joback Method
dvisc	0.0000282	Pa×s	816.39	Joback Method
dvisc	0.0000386	Pa×s	759.13	Joback Method
dvisc	0.0000556	Pa×s	701.87	Joback Method
dvisc	0.0000855	Pa×s	644.60	Joback Method
dvisc	0.0001430	Pa×s	587.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117851&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
mccvol:	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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