Diethylene glycol monobenzoate

Other names: 2-(2-hydroxyethoxy)ethyl benzoate
Inchi: InChI=1S/C11H14O4/c12-6-7-14-8-9-15-11(13)10-4-2-1-3-5-10/h1-5,12H,6-9H2
InchiKey: DNUPYEDSAQDUSO-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: O=C(OCCOCCO)c1ccccc1
Mol. weight [g/mol]: 210.23
CAS: 20587-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-321.59	kJ/mol	Joback Method
hf	-563.09	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.852		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	668.65	K	Joback Method
tc	863.43	K	Joback Method
tf	395.36	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.70	J/mol×K	668.65	Joback Method
cpg	436.35	J/mol×K	701.11	Joback Method
cpg	447.33	J/mol×K	733.58	Joback Method
cpg	457.64	J/mol×K	766.04	Joback Method
cpg	467.30	J/mol×K	798.50	Joback Method
cpg	476.31	J/mol×K	830.97	Joback Method
cpg	484.67	J/mol×K	863.43	Joback Method
dvisc	0.0017511	Pa×s	395.36	Joback Method

dvisc	0.0006854	Pa×s	440.91	Joback Method
dvisc	0.0003198	Pa×s	486.46	Joback Method
dvisc	0.0001700	Pa×s	532.00	Joback Method
dvisc	0.0000999	Pa×s	577.55	Joback Method
dvisc	0.0000634	Pa×s	623.10	Joback Method
dvisc	0.0000428	Pa×s	668.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20587615&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