

Benzoic acid 4-ethoxy-2-ethoxymethyl-5-methoxy-tetrahydro-pyran-3-yl ester

Inchi:	InChI=1S/C18H26O6/c1-4-21-11-13-9-17(23-5-2)16(20-3)10-15(13)18(19)24-14-7-6-8-22
InchiKey:	PNUWFVSMBQWHQC-UHFFFAOYSA-N
Formula:	C18H26O6
SMILES:	CCOCc1cc(OCC)c(OC)cc1C(=O)OC1CCCOC1
Mol. weight [g/mol]:	338.40

Physical Properties

Property code	Value	Unit	Source
gf	-426.39	kJ/mol	Joback Method
hf	-931.87	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.966		Crippen Method
mvol	260.780	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2105.26		NIST Webbook
rinpol	2143.99		NIST Webbook
tb	842.91	K	Joback Method
tc	1058.34	K	Joback Method
tf	529.40	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.91	J/molxK	842.91	Joback Method
cpg	843.42	J/molxK	878.82	Joback Method
cpg	858.43	J/molxK	914.72	Joback Method
cpg	871.92	J/molxK	950.63	Joback Method
cpg	883.86	J/molxK	986.53	Joback Method
cpg	894.23	J/molxK	1022.44	Joback Method
cpg	903.02	J/molxK	1058.34	Joback Method
dvisc	0.0003145	Paxs	529.40	Joback Method

dvisc	0.0001900	Paxs	581.65	Joback Method
dvisc	0.0001247	Paxs	633.90	Joback Method
dvisc	0.0000873	Paxs	686.15	Joback Method
dvisc	0.0000643	Paxs	738.41	Joback Method
dvisc	0.0000493	Paxs	790.66	Joback Method
dvisc	0.0000390	Paxs	842.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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