Fenproporex-M (desamino-oxo-di-HO), 2AC

Inchi: InChI=1S/C13H14O5/c1-8(14)6-11-4-5-12(17-9(2)15)7-13(11)18-10(3)16/h4-5,7H,6H2,1-
InchiKey: FRVVDNILXRUHSD-UHFFFAOYSA-N
Formula: C13H14O5
SMILES: CC(=O)Cc1ccc(OC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
gf	-445.03	kJ/mol	Joback Method
hf	-700.24	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	73.19	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.669		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	739.93	K	Joback Method
tc	955.63	K	Joback Method
tf	481.98	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.73	J/mol×K	739.93	Joback Method
cpg	553.27	J/mol×K	919.68	Joback Method
cpg	544.56	J/mol×K	883.73	Joback Method
cpg	534.94	J/mol×K	847.78	Joback Method
cpg	524.42	J/mol×K	811.83	Joback Method
cpg	513.02	J/mol×K	775.88	Joback Method
cpg	561.08	J/mol×K	955.63	Joback Method
dvisc	0.0001338	Pa×s	739.93	Joback Method

dvisc	0.0001641	Pa×s	696.94	Joback Method
dvisc	0.0002068	Pa×s	653.95	Joback Method
dvisc	0.0002691	Pa×s	610.96	Joback Method
dvisc	0.0003645	Pa×s	567.96	Joback Method
dvisc	0.0005187	Pa×s	524.97	Joback Method
dvisc	0.0007863	Pa×s	481.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R275097&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