2-Phenoxyethyl caproate

Inchi: InChI=1S/C14H20O3/c1-2-3-5-10-14(15)17-12-11-16-13-8-6-4-7-9-13/h4,6-9H,2-3,5,10-1
InchiKey: KPKMFOVQBMXMOI-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: CCCCCC(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	-159.51	kJ/mol	Joback Method
hf	-472.78	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	60.60	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.189		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	645.11	K	Joback Method
tc	843.53	K	Joback Method
tf	368.35	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.43	J/mol×K	645.11	Joback Method
cpg	592.68	J/mol×K	810.46	Joback Method
cpg	580.13	J/mol×K	777.39	Joback Method
cpg	566.74	J/mol×K	744.32	Joback Method
cpg	552.51	J/mol×K	711.25	Joback Method
cpg	537.41	J/mol×K	678.18	Joback Method
cpg	604.40	J/mol×K	843.53	Joback Method
dvisc	0.0001194	Pa×s	645.11	Joback Method

dvisc	0.0001543	Pa×s	598.98	Joback Method
dvisc	0.0002083	Pa×s	552.86	Joback Method
dvisc	0.0002969	Pa×s	506.73	Joback Method
dvisc	0.0004543	Pa×s	460.60	Joback Method
dvisc	0.0007642	Pa×s	414.48	Joback Method
dvisc	0.0014644	Pa×s	368.35	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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