2-Ethylbutyric acid, 3-phenoxybenzyl ester

Inchi: InChI=1S/C19H22O3/c1-3-16(4-2)19(20)21-14-15-9-8-12-18(13-15)22-17-10-6-5-7-11-17
InchiKey: SJIRZDFDZYLLLH-UHFFFAOYSA-N
Formula: C19H22O3
SMILES: CCC(CC)C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 298.38

Physical Properties

Property code	Value	Unit	Source
gf	-17.07	kJ/mol	Joback Method
hf	-356.20	kJ/mol	Joback Method
hfus	33.11	kJ/mol	Joback Method
hvap	74.28	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.958		Crippen Method
mcvol	244.360	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2196.00		NIST Webbook
tb	790.73	K	Joback Method
tc	1014.28	K	Joback Method
tf	448.64	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.10	J/mol×K	790.73	Joback Method
cpg	726.50	J/mol×K	827.99	Joback Method
cpg	741.60	J/mol×K	865.25	Joback Method
cpg	755.44	J/mol×K	902.51	Joback Method
cpg	768.08	J/mol×K	939.76	Joback Method
cpg	779.53	J/mol×K	977.02	Joback Method
cpg	789.84	J/mol×K	1014.28	Joback Method
dvisc	0.0007740	Pa×s	448.64	Joback Method
dvisc	0.0003983	Pa×s	505.66	Joback Method

dvisc	0.0002345	Pa×s	562.67	Joback Method
dvisc	0.0001522	Pa×s	619.69	Joback Method
dvisc	0.0001063	Pa×s	676.70	Joback Method
dvisc	0.0000784	Pa×s	733.72	Joback Method
dvisc	0.0000605	Pa×s	790.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370238&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
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