3-Phenoxybenzyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C18H18O3/c1-3-14(2)18(19)20-13-15-8-7-11-17(12-15)21-16-9-5-4-6-10-16/h3
InchiKey: PTDIDLMUDYYUQZ-LZWSPWQCSA-N
Formula: C18H18O3
SMILES: CC=C(C)C(=O)OCc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 282.33

Physical Properties

Property code	Value	Unit	Source
gf	48.62	kJ/mol	Joback Method
hf	-222.85	kJ/mol	Joback Method
hfus	32.94	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.488		Crippen Method
mcvol	225.970	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	2233.00		NIST Webbook
rinpol	2233.00		NIST Webbook
tb	772.33	K	Joback Method
tc	1006.56	K	Joback Method
tf	433.33	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.09	J/mol×K	772.33	Joback Method
cpg	643.77	J/mol×K	811.37	Joback Method
cpg	658.20	J/mol×K	850.41	Joback Method
cpg	671.45	J/mol×K	889.44	Joback Method
cpg	683.57	J/mol×K	928.48	Joback Method
cpg	694.62	J/mol×K	967.52	Joback Method
cpg	704.66	J/mol×K	1006.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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