OXetane, 3-bromomethyl-3-phenoxymethyl

Inchi: InChI=1S/C11H13BrO2/c12-6-11(7-13-8-11)9-14-10-4-2-1-3-5-10/h1-5H,6-9H2
InchiKey: QTLNADFKGYFMEL-UHFFFAOYSA-N
Formula: C11H13BrO2
SMILES: BrCC1(COc2ccccc2)COC1
Mol. weight [g/mol]: 257.12

Physical Properties

Property code	Value	Unit	Source
gf	20.51	kJ/mol	Joback Method
hf	-189.85	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	54.64	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.477		Crippen Method
mcvol	160.470	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	604.54	K	Joback Method
tc	850.28	K	Joback Method
tf	387.07	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.69	J/mol×K	604.54	Joback Method
cpg	397.77	J/mol×K	645.50	Joback Method
cpg	411.76	J/mol×K	686.45	Joback Method
cpg	424.87	J/mol×K	727.41	Joback Method
cpg	437.30	J/mol×K	768.37	Joback Method
cpg	449.24	J/mol×K	809.33	Joback Method
cpg	460.89	J/mol×K	850.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6667&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
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