2-Bromopropionic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C16H15BrO3/c1-12(17)16(18)20-15-9-7-14(8-10-15)19-11-13-5-3-2-4-6-13/h2-

InchiKey: YUOYIAWWHSMJSH-UHFFFAOYSA-N

Formula: C16H15BrO3

SMILES: CC(Br)C(=O)Oc1ccc(OCc2ccccc2)cc1

Mol. weight [g/mol]: 335.19

Physical Properties

Property code	Value	Unit	Source
gf	-28.01	kJ/mol	Joback Method
hf	-267.95	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	74.04	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.954		Crippen Method
mcvol	219.590	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	788.25	K	Joback Method
tc	1032.80	K	Joback Method
tf	474.63	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.58	J/mol×K	788.25	Joback Method
cpg	595.41	J/mol×K	829.01	Joback Method
cpg	607.98	J/mol×K	869.77	Joback Method
cpg	619.35	J/mol×K	910.53	Joback Method
cpg	629.56	J/mol×K	951.29	Joback Method
cpg	638.67	J/mol×K	992.04	Joback Method
cpg	646.72	J/mol×K	1032.80	Joback Method
dvisc	0.0006848	Pa×s	474.63	Joback Method

dvisc	0.0003939	Pa×s	526.90	Joback Method
dvisc	0.0002504	Pa×s	579.17	Joback Method
dvisc	0.0001716	Pa×s	631.44	Joback Method
dvisc	0.0001245	Pa×s	683.71	Joback Method
dvisc	0.0000946	Pa×s	735.98	Joback Method
dvisc	0.0000745	Pa×s	788.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308029&Units=SI

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