2-Ethylbutyric acid, 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C13H17BrO3/c1-4-9(5-2)13(15)17-11-7-6-10(14)8-12(11)16-3/h6-9H,4-5H2,1-3

InchiKey: DJJDARBLXWGICA-UHFFFAOYSA-N

Formula: C13H17BrO3

SMILES: CCC(CC)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 301.18

Physical Properties

Property code	Value	Unit	Source
gf	-175.31	kJ/mol	Joback Method
hf	-454.03	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.799		Crippen Method
mcvol	201.080	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1838.00		NIST Webbook
tb	697.91	K	Joback Method
tc	915.61	K	Joback Method
tf	426.92	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.91	J/mol×K	697.91	Joback Method
cpg	571.78	J/mol×K	879.32	Joback Method
cpg	561.15	J/mol×K	843.04	Joback Method
cpg	549.66	J/mol×K	806.76	Joback Method
cpg	537.29	J/mol×K	770.48	Joback Method
cpg	524.05	J/mol×K	734.19	Joback Method
cpg	581.55	J/mol×K	915.61	Joback Method
dvisc	0.0001086	Pa×s	697.91	Joback Method
dvisc	0.0001361	Pa×s	652.75	Joback Method

dvisc	0.0001765	Pa×s	607.58	Joback Method
dvisc	0.0002385	Pa×s	562.41	Joback Method
dvisc	0.0003397	Pa×s	517.25	Joback Method
dvisc	0.0005177	Pa×s	472.09	Joback Method
dvisc	0.0008627	Pa×s	426.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U371167&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
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