Fumaric acid, monoamide, N-(2-bromophenyl)-, pentafluorobenzyl ester

Inchi: InChI=1S/C17H9BrF5NO3/c18-9-3-1-2-4-10(9)24-11(25)5-6-12(26)27-7-8-13(19)15(21)1

InchiKey: MQVQSVSRYMMRCP-AATRIKPKSA-N

Formula: C17H9BrF5NO3

SMILES: O=C(C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)Nc1ccccc1Br

Mol. weight [g/mol]: 450.15

Physical Properties

Property code	Value	Unit	Source
gf	-893.66	kJ/mol	Joback Method
hf	-1130.88	kJ/mol	Joback Method
hfus	55.91	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.383		Crippen Method
mcvol	243.910	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	918.60	K	Joback Method
tc	1138.42	K	Joback Method
tf	641.73	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.10	J/mol×K	918.60	Joback Method
cpg	678.80	J/mol×K	955.24	Joback Method
cpg	686.70	J/mol×K	991.87	Joback Method
cpg	693.85	J/mol×K	1028.51	Joback Method
cpg	700.27	J/mol×K	1065.15	Joback Method
cpg	706.02	J/mol×K	1101.79	Joback Method
cpg	711.13	J/mol×K	1138.42	Joback Method

Sources

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=U357451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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