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

Inchi: InChI=1S/C18H24BrNO3/c1-3-5-8-14(4-2)13-23-18(22)12-11-17(21)20-16-10-7-6-9-15(1

InchiKey: SEWPTVMMOJRPFC-VAWYXSNFSA-N

Formula: C18H24BrNO3

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Nc1ccccc1Br

Mol. weight [g/mol]: 382.29

Physical Properties

Property code	Value	Unit	Source
gf	22.11	kJ/mol	Joback Method
hf	-355.43	kJ/mol	Joback Method
hfus	47.48	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.703		Crippen Method
mcvol	272.910	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	2780.00		NIST Webbook
tb	893.11	K	Joback Method
tc	1113.24	K	Joback Method
tf	546.03	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.22	J/mol×K	893.11	Joback Method
cpg	815.70	J/mol×K	929.80	Joback Method
cpg	828.21	J/mol×K	966.49	Joback Method
cpg	839.83	J/mol×K	1003.17	Joback Method
cpg	850.61	J/mol×K	1039.86	Joback Method
cpg	860.62	J/mol×K	1076.55	Joback Method
cpg	869.93	J/mol×K	1113.24	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=U357508&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