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

Inchi: InChI=1S/C15H18BrNO3/c1-3-6-11(2)20-15(19)10-9-14(18)17-13-8-5-4-7-12(13)16/h4-5

InchiKey: YZPLUFJJPUGYDS-MDZDMXLPSA-N

Formula: C15H18BrNO3

SMILES: CCCC(C)OC(=O)C=CC(=O)Nc1ccccc1Br

Mol. weight [g/mol]: 340.21

Physical Properties

Property code	Value	Unit	Source
gf	-3.15	kJ/mol	Joback Method
hf	-293.51	kJ/mol	Joback Method
hfus	39.71	kJ/mol	Joback Method
hvap	80.27	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.676		Crippen Method
mcvol	230.640	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	824.47	K	Joback Method
tc	1049.78	K	Joback Method
tf	512.22	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.87	J/mol×K	824.47	Joback Method
cpg	645.45	J/mol×K	862.02	Joback Method
cpg	657.10	J/mol×K	899.57	Joback Method
cpg	667.86	J/mol×K	937.13	Joback Method
cpg	677.81	J/mol×K	974.68	Joback Method
cpg	686.99	J/mol×K	1012.23	Joback Method
cpg	695.48	J/mol×K	1049.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357496&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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