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

Inchi: InChI=1S/C15H18BrNO3/c1-15(2,3)10-20-14(19)9-8-13(18)17-12-7-5-4-6-11(12)16/h4-9
InchiKey: IIKYRXUQHOAFHV-CMDGGOBGSA-N
Formula: C15H18BrNO3
SMILES: CC(C)(C)COC(=O)C=CC(=O)Nc1ccccc1Br
Mol. weight [g/mol]: 340.21

Physical Properties

Property code	Value	Unit	Source
gf	2.13	kJ/mol	Joback Method
hf	-296.98	kJ/mol	Joback Method
hfus	35.82	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.533		Crippen Method
mcvol	230.640	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	821.68	K	Joback Method
tc	1053.41	K	Joback Method
tf	529.64	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.97	J/mol×K	821.68	Joback Method
cpg	646.59	J/mol×K	860.30	Joback Method
cpg	658.26	J/mol×K	898.92	Joback Method
cpg	669.08	J/mol×K	937.55	Joback Method
cpg	679.14	J/mol×K	976.17	Joback Method
cpg	688.53	J/mol×K	1014.79	Joback Method
cpg	697.34	J/mol×K	1053.41	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=U357515&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