Fumaric acid, monoamide, N-(2-bromophenyl)-, 3,5-difluorophenyl ester

Other names: Fumaric acid, monoamide, N-(2-bromophenyl)-, 3,5-fluorophenyl ester
Inchi: InChI=1S/C16H10BrF2NO3/c17-13-3-1-2-4-14(13)20-15(21)5-6-16(22)23-12-8-10(18)7-1
InchiKey: IDSBBDZGAFTYLY-AATRIKPKSA-N
Formula: C16H10BrF2NO3
SMILES: O=C(C=CC(=O)Oc1cc(F)cc(F)c1)Nc1ccccc1Br
Mol. weight [g/mol]: 382.16

Physical Properties

Property code	Value	Unit	Source
gf	-288.76	kJ/mol	Joback Method
hf	-487.50	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.828		Crippen Method
mcvol	224.510	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	882.97	K	Joback Method
tc	1120.65	K	Joback Method
tf	591.13	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.68	J/mol×K	882.97	Joback Method
cpg	608.32	J/mol×K	922.58	Joback Method
cpg	617.08	J/mol×K	962.20	Joback Method
cpg	625.02	J/mol×K	1001.81	Joback Method
cpg	632.21	J/mol×K	1041.43	Joback Method
cpg	638.73	J/mol×K	1081.04	Joback Method
cpg	644.64	J/mol×K	1120.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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