Fumaric acid, 4-bromophenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H9BrF8O4/c16-8-1-3-9(4-2-8)28-11(26)6-5-10(25)27-7-13(19,20)15(23,24)14(21,22)12(17)18/h1-6,12H,7H2/b6-5-

InchiKey: AZFUITGMYJGTHK-AATRIKPKSA-N

Formula: C15H9BrF8O4

SMILES: O=C(C=CC(=O)Oc1ccc(Br)cc1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 485.12

Physical Properties

Property code	Value	Unit	Source
gf	-1747.50	kJ/mol	Joback Method
hf	-2074.33	kJ/mol	Joback Method
hfus	38.19	kJ/mol	Joback Method
hvap	65.81	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.625		Crippen Method
mcvol	240.690	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2031.00		NIST Webbook
tb	781.19	K	Joback Method
tc	976.03	K	Joback Method
tf	493.77	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.64	J/mol×K	781.19	Joback Method
cpg	684.25	J/mol×K	813.66	Joback Method
cpg	693.07	J/mol×K	846.14	Joback Method
cpg	701.19	J/mol×K	878.61	Joback Method
cpg	708.69	J/mol×K	911.09	Joback Method
cpg	715.64	J/mol×K	943.56	Joback Method
cpg	722.13	J/mol×K	976.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405765&Units=SI

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