Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C16H12BrF9O4/c17-9-6-8(18)4-5-10(9)30-12(28)3-1-2-11(27)29-7-14(21,22)16

InchiKey: YFJSGDXHRUHVTF-UHFFFAOYSA-N

Formula: C16H12BrF9O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)cc1Br)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 519.15

Physical Properties

Property code	Value	Unit	Source
gf	-2023.74	kJ/mol	Joback Method
hf	-2419.77	kJ/mol	Joback Method
hfus	43.27	kJ/mol	Joback Method
hvap	67.93	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.378		Crippen Method
mcvol	260.850	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	804.16	K	Joback Method
tc	992.31	K	Joback Method
tf	523.23	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.40	J/mol×K	804.16	Joback Method
cpg	770.65	J/mol×K	835.52	Joback Method
cpg	780.11	J/mol×K	866.88	Joback Method
cpg	788.84	J/mol×K	898.24	Joback Method
cpg	796.90	J/mol×K	929.59	Joback Method
cpg	804.35	J/mol×K	960.95	Joback Method
cpg	811.25	J/mol×K	992.31	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=U391823&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