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

Inchi: InChI=1S/C17H15BrF8O5/c1-29-11-7-9(18)5-6-10(11)31-13(28)4-2-3-12(27)30-8-15(21,2

InchiKey: OIBYHBWBUGCNDD-UHFFFAOYSA-N

Formula: C17H15BrF8O5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 531.19

Physical Properties

Property code	Value	Unit	Source
gf	-1925.51	kJ/mol	Joback Method
hf	-2376.52	kJ/mol	Joback Method
hfus	43.97	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.248		Crippen Method
mcvol	279.040	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2274.00		NIST Webbook
tb	850.19	K	Joback Method
tc	1045.53	K	Joback Method
tf	556.14	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.66	J/mol×K	850.19	Joback Method
cpg	844.31	J/mol×K	882.75	Joback Method
cpg	854.10	J/mol×K	915.30	Joback Method
cpg	863.07	J/mol×K	947.86	Joback Method
cpg	871.28	J/mol×K	980.41	Joback Method
cpg	878.80	J/mol×K	1012.97	Joback Method
cpg	885.67	J/mol×K	1045.53	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=U393656&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