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

Inchi: InChI=1S/C16H13BrF8O4/c17-9-4-6-10(7-5-9)29-12(27)3-1-2-11(26)28-8-14(20,21)16(24

InchiKey: XNERHNYDEGZQGY-UHFFFAOYSA-N

Formula: C16H13BrF8O4

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

Mol. weight [g/mol]: 501.16

Physical Properties

Property code	Value	Unit	Source
gf	-1819.30	kJ/mol	Joback Method
hf	-2212.19	kJ/mol	Joback Method
hfus	40.58	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.239		Crippen Method
mcvol	259.080	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	799.91	K	Joback Method
tc	990.80	K	Joback Method
tf	510.12	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.19	J/mol×K	799.91	Joback Method
cpg	764.81	J/mol×K	831.72	Joback Method
cpg	774.61	J/mol×K	863.54	Joback Method
cpg	783.64	J/mol×K	895.35	Joback Method
cpg	791.99	J/mol×K	927.17	Joback Method
cpg	799.70	J/mol×K	958.98	Joback Method
cpg	806.86	J/mol×K	990.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393284&Units=SI
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

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