Glutaric acid, 2-bromo-5-fluorobenzyl hexyl ester

Inchi: InChI=1S/C18H24BrFO4/c1-2-3-4-5-11-23-17(21)7-6-8-18(22)24-13-14-12-15(20)9-10-1

InchiKey: XNEFJYJJKSLNFS-UHFFFAOYSA-N

Formula: C18H24BrFO4

SMILES: CCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 403.28

Physical Properties

Property code	Value	Unit	Source
gf	-454.50	kJ/mol	Joback Method
hf	-860.64	kJ/mol	Joback Method
hfus	49.58	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.925		Crippen Method
mcvol	274.870	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	865.89	K	Joback Method
tc	1072.39	K	Joback Method
tf	548.79	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.56	J/mol×K	865.89	Joback Method
cpg	821.09	J/mol×K	900.31	Joback Method
cpg	833.59	J/mol×K	934.72	Joback Method
cpg	845.08	J/mol×K	969.14	Joback Method
cpg	855.58	J/mol×K	1003.56	Joback Method
cpg	865.11	J/mol×K	1037.98	Joback Method
cpg	873.70	J/mol×K	1072.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377065&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