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

Inchi: InChI=1S/C19H26BrFO4/c1-2-3-4-5-6-12-24-18(22)8-7-9-19(23)25-14-15-13-16(21)10-1

InchiKey: RPAFONNINAFYJS-UHFFFAOYSA-N

Formula: C19H26BrFO4

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

Mol. weight [g/mol]: 417.31

Physical Properties

Property code	Value	Unit	Source
gf	-446.08	kJ/mol	Joback Method
hf	-881.28	kJ/mol	Joback Method
hfus	52.17	kJ/mol	Joback Method
hvap	85.42	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.315		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	888.77	K	Joback Method
tc	1096.25	K	Joback Method
tf	560.06	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.58	J/mol×K	888.77	Joback Method
cpg	879.37	J/mol×K	923.35	Joback Method
cpg	892.08	J/mol×K	957.93	Joback Method
cpg	903.74	J/mol×K	992.51	Joback Method
cpg	914.37	J/mol×K	1027.09	Joback Method
cpg	924.00	J/mol×K	1061.67	Joback Method
cpg	932.65	J/mol×K	1096.25	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=U377066&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