Glutaric acid, 2-ethylhexyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C19H26BrFO4/c1-3-5-7-14(4-2)13-24-18(22)8-6-9-19(23)25-17-11-10-15(21)1

InchiKey: XVOUPLFDTFLFAW-UHFFFAOYSA-N

Formula: C19H26BrFO4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 417.31

Physical Properties

Property code	Value	Unit	Source
gf	-448.52	kJ/mol	Joback Method
hf	-886.56	kJ/mol	Joback Method
hfus	48.64	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.423		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	888.33	K	Joback Method
tc	1097.32	K	Joback Method
tf	545.06	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.10	J/mol×K	888.33	Joback Method
cpg	879.96	J/mol×K	923.16	Joback Method
cpg	892.72	J/mol×K	957.99	Joback Method
cpg	904.39	J/mol×K	992.82	Joback Method
cpg	915.02	J/mol×K	1027.65	Joback Method
cpg	924.61	J/mol×K	1062.49	Joback Method
cpg	933.20	J/mol×K	1097.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391832&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

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