Glutaric acid, hex-4-yn-3-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C17H18BrFO4/c1-3-6-13(4-2)22-16(20)7-5-8-17(21)23-15-10-9-12(19)11-14(15

InchiKey: DXLZEELVIOBDIJ-UHFFFAOYSA-N

Formula: C17H18BrFO4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 385.23

Physical Properties

Property code	Value	Unit	Source
gf	-262.56	kJ/mol	Joback Method
hf	-572.98	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	82.73	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.009		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	851.57	K	Joback Method
tc	1074.92	K	Joback Method
tf	628.62	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.29	J/mol×K	851.57	Joback Method
cpg	710.92	J/mol×K	888.79	Joback Method
cpg	722.48	J/mol×K	926.02	Joback Method
cpg	732.99	J/mol×K	963.24	Joback Method
cpg	742.48	J/mol×K	1000.47	Joback Method
cpg	750.95	J/mol×K	1037.69	Joback Method
cpg	758.42	J/mol×K	1074.92	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=U389753&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