

Glutaric acid, 2,6-difluoro-4-bromobenzyl ethyl ester

Inchi:	InChI=1S/C14H15BrF2O4/c1-2-20-13(18)4-3-5-14(19)21-8-10-11(16)6-9(15)7-12(10)17/
InchiKey:	ADXMZGHFVFKNJ-UHFFFAOYSA-N
Formula:	C14H15BrF2O4
SMILES:	CCOC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]:	365.17

Physical Properties

Property code	Value	Unit	Source
gf	-692.62	kJ/mol	Joback Method
hf	-985.66	kJ/mol	Joback Method
hfus	41.91	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.504		Crippen Method
mcvol	220.280	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpola	2084.00		NIST Webbook
tb	778.62	K	Joback Method
tc	982.21	K	Joback Method
tf	516.82	K	Joback Method
vc	0.858	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.52	J/molxK	778.62	Joback Method
cpg	602.21	J/molxK	812.55	Joback Method
cpg	613.08	J/molxK	846.48	Joback Method
cpg	623.14	J/molxK	880.42	Joback Method
cpg	632.39	J/molxK	914.35	Joback Method
cpg	640.85	J/molxK	948.28	Joback Method
cpg	648.51	J/molxK	982.21	Joback Method

Sources

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=U376816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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