

Glutaric acid, 3,4-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C16H20F2O4/c1-11(2)9-21-15(19)4-3-5-16(20)22-10-12-6-7-13(17)14(18)8-12
InchiKey: NQWZPRDIWNTFTP-UHFFFAOYSA-N
Formula: C16H20F2O4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 314.32

Physical Properties

Property code	Value	Unit	Source
gf	-682.91	kJ/mol	Joback Method
hf	-1047.08	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.377		Crippen Method
mvol	230.960	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2207.00		NIST Webbook
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tb	752.80	K	Joback Method
tc	945.68	K	Joback Method
tf	452.04	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.63	J/molxK	752.80	Joback Method
cpg	677.78	J/molxK	784.95	Joback Method
cpg	691.04	J/molxK	817.09	Joback Method
cpg	703.41	J/molxK	849.24	Joback Method
cpg	714.91	J/molxK	881.39	Joback Method
cpg	725.55	J/molxK	913.53	Joback Method
cpg	735.32	J/molxK	945.68	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=U377634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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