

Glutaric acid, di(2-fluorobenzyl) ester

Inchi: InChI=1S/C19H18F2O4/c20-16-8-3-1-6-14(16)12-24-18(22)10-5-11-19(23)25-13-15-7-2-
InchiKey: AWUCHWCQMSULEN-UHFFFAOYSA-N
Formula: C19H18F2O4
SMILES: O=C(CCCC(=O)OCc1ccccc1F)OCc1ccccc1F
Mol. weight [g/mol]: 348.34

Physical Properties

Property code	Value	Unit	Source
gf	-542.80	kJ/mol	Joback Method
hf	-867.19	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.922		Crippen Method
mvol	249.470	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	848.56	K	Joback Method
tc	1062.01	K	Joback Method
tf	527.27	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.08	J/mol×K	848.56	Joback Method
cpg	751.06	J/mol×K	884.14	Joback Method
cpg	762.90	J/mol×K	919.71	Joback Method
cpg	773.64	J/mol×K	955.29	Joback Method
cpg	783.29	J/mol×K	990.86	Joback Method
cpg	791.90	J/mol×K	1026.44	Joback Method
cpg	799.48	J/mol×K	1062.01	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=U377675&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
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

Latest version available from:

<https://www.cheméo.com/cid/116-770-8/Glutaric-acid-di-2-fluorobenzyl-ester.pdf>

Generated by Cheméo on 2024-05-01 14:44:53.406069839 +0000 UTC m=+16863942.326647162.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.