

Glutaric acid, 3,5-difluorophenyl nonyl ester

Inchi:	InChI=1S/C20H28F2O4/c1-2-3-4-5-6-7-8-12-25-19(23)10-9-11-20(24)26-18-14-16(21)13
InchiKey:	JWQLMNFPTPLPJM-UHFFFAOYSA-N
Formula:	C20H28F2O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	370.43

Physical Properties

Property code	Value	Unit	Source
gf	-646.79	kJ/mol	Joback Method
hf	-1124.36	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.334		Crippen Method
mvol	287.320	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	844.76	K	Joback Method
tc	1038.99	K	Joback Method
tf	512.12	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.79	J/molxK	844.76	Joback Method
cpg	907.11	J/molxK	877.13	Joback Method
cpg	921.37	J/molxK	909.50	Joback Method
cpg	934.58	J/molxK	941.87	Joback Method
cpg	946.76	J/molxK	974.24	Joback Method
cpg	957.92	J/molxK	1006.62	Joback Method
cpg	968.09	J/molxK	1038.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358634&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

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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