

Glutaric acid, nonyl 4-(trifluoromethyl)benzyl ester

Inchi:	InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-16-28-20(26)10-9-11-21(27)29-17-18-12-14-19
InchiKey:	RWALQSCLSMUCIM-UHFFFAOYSA-N
Formula:	C22H31F3O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	416.47

Physical Properties

Property code	Value	Unit	Source
gf	-812.29	kJ/mol	Joback Method
hf	-1359.03	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.213		Crippen Method
mvol	317.270	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2739.00		NIST Webbook
rinpol	2739.00		NIST Webbook
tb	881.58	K	Joback Method
tc	1080.54	K	Joback Method
tf	525.15	K	Joback Method
vc	1.250	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.44	J/molxK	881.58	Joback Method
cpg	1035.16	J/molxK	914.74	Joback Method
cpg	1049.75	J/molxK	947.90	Joback Method
cpg	1063.24	J/molxK	981.06	Joback Method
cpg	1075.70	J/molxK	1014.22	Joback Method
cpg	1087.16	J/molxK	1047.38	Joback Method
cpg	1097.67	J/molxK	1080.54	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=U377584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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