

Glutaric acid, 1-phenyl-2,2,2-trifluoroethyl tridecyl ester

Inchi:	InChI=1S/C26H39F3O4/c1-2-3-4-5-6-7-8-9-10-11-15-21-32-23(30)19-16-20-24(31)33-25
InchiKey:	ZMRVZELXFBOKQT-UHFFFAOYSA-N
Formula:	C26H39F3O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	472.58

Physical Properties

Property code	Value	Unit	Source
gf	-771.42	kJ/mol	Joback Method
hf	-1435.40	kJ/mol	Joback Method
hfus	61.01	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.858		Crippen Method
mcvol	373.630	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpola	2891.00		NIST Webbook
tb	967.68	K	Joback Method
tc	1186.64	K	Joback Method
tf	542.71	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.02	J/molxK	967.68	Joback Method
cpg	1282.33	J/molxK	1004.17	Joback Method
cpg	1298.23	J/molxK	1040.67	Joback Method
cpg	1312.80	J/molxK	1077.16	Joback Method
cpg	1326.12	J/molxK	1113.65	Joback Method
cpg	1338.28	J/molxK	1150.14	Joback Method
cpg	1349.36	J/molxK	1186.64	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=U377375&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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