

Glutaric acid, pentadecyl 4-(trifluoromethoxy)benzyl ester

Inchi:	InChI=1S/C28H43F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-22-34-26(32)16-15-17-27(33)
InchiKey:	JUYAVASXWMJLW-UHFFFAOYSA-N
Formula:	C28H43F3O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	516.63

Physical Properties

Property code	Value	Unit	Source
gf	-866.77	kJ/mol	Joback Method
hf	-1615.09	kJ/mol	Joback Method
hfus	70.52	kJ/mol	Joback Method
hvap	97.83	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.433		Crippen Method
mvol	407.680	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	3182.00		NIST Webbook
rinpol	3182.00		NIST Webbook
tb	1041.28	K	Joback Method
tc	1290.49	K	Joback Method
tf	615.00	K	Joback Method
vc	1.605	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.08	J/molxK	1041.28	Joback Method
cpg	1435.69	J/molxK	1082.82	Joback Method
cpg	1451.33	J/molxK	1124.35	Joback Method
cpg	1465.10	J/molxK	1165.89	Joback Method
cpg	1477.10	J/molxK	1207.42	Joback Method
cpg	1487.42	J/molxK	1248.96	Joback Method
cpg	1496.17	J/molxK	1290.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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