Glutaric acid, 1,1,1-trifluoroprop-2-yl dodecyl ester

Inchi: InChI=1S/C20H35F3O4/c1-3-4-5-6-7-8-9-10-11-12-16-26-18(24)14-13-15-19(25)27-17(2

InchiKey: VXKVKGVGRLXIJL-UHFFFAOYSA-N

Formula: C20H35F3O4

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-934.35	kJ/mol	Joback Method
hf	-1548.09	kJ/mol	Joback Method
hfus	51.43	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.115		Crippen Method
mcvol	312.850	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	803.72	K	Joback Method
tc	984.66	K	Joback Method
tf	448.67	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.95	J/mol×K	803.72	Joback Method
cpg	1010.45	J/mol×K	833.88	Joback Method
cpg	1026.93	J/mol×K	864.03	Joback Method
cpg	1042.42	J/mol×K	894.19	Joback Method
cpg	1056.95	J/mol×K	924.34	Joback Method
cpg	1070.56	J/mol×K	954.50	Joback Method
cpg	1083.27	J/mol×K	984.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391594&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
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
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
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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