Succinic acid, tetradecyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C20H35F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-26-18(24)14-15-19(25)27-17
InchiKey: PMBZIWOOTVFXRK-UHFFFAOYSA-N
Formula: C20H35F3O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-931.91	kJ/mol	Joback Method
hf	-1542.81	kJ/mol	Joback Method
hfus	54.96	kJ/mol	Joback Method
hvap	74.68	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.116		Crippen Method
mcvol	312.850	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	804.16	K	Joback Method
tc	984.84	K	Joback Method
tf	463.67	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.47	J/mol×K	804.16	Joback Method
cpg	1009.94	J/mol×K	834.27	Joback Method
cpg	1026.40	J/mol×K	864.39	Joback Method
cpg	1041.88	J/mol×K	894.50	Joback Method
cpg	1056.42	J/mol×K	924.61	Joback Method
cpg	1070.04	J/mol×K	954.73	Joback Method
cpg	1082.78	J/mol×K	984.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382472&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
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