Sebacic acid, decyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C28H43F3O5/c1-2-3-4-5-6-9-12-15-22-34-26(32)16-13-10-7-8-11-14-17-27(33

InchiKey: VDPJSINRKDCJHO-UHFFFAOYSA-N

Formula: C28H43F3O5

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=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
mcvol	407.680	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	1041.28	K	Joback Method
tc	1290.49	K	Joback Method
tf	615.00	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416797&Units=SI

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