2,5-Di(trifluoromethyl)benzoic acid, pentadecyl ester

Inchi: InChI=1S/C24H34F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-32-22(31)20-18-19(23(25

InchiKey: OQAGOVODWOBRMN-UHFFFAOYSA-N

Formula: C24H34F6O2

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 468.52

Physical Properties

Property code	Value	Unit	Source
gf	-1152.75	kJ/mol	Joback Method
hf	-1764.06	kJ/mol	Joback Method
hfus	57.62	kJ/mol	Joback Method
hvap	74.28	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.972		Crippen Method
mcvol	343.320	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	2326.00		NIST Webbook
rinpol	2326.00		NIST Webbook
tb	850.61	K	Joback Method
tc	1041.39	K	Joback Method
tf	492.24	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.05	J/mol×K	850.61	Joback Method
cpg	1129.60	J/mol×K	882.41	Joback Method
cpg	1146.09	J/mol×K	914.20	Joback Method
cpg	1161.57	J/mol×K	946.00	Joback Method
cpg	1176.13	J/mol×K	977.80	Joback Method
cpg	1189.83	J/mol×K	1009.59	Joback Method
cpg	1202.74	J/mol×K	1041.39	Joback Method

Sources

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=U338948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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