2,5-Di(trifluoromethyl)benzoic acid, 6-pentadecyl ester

Inchi: InChI=1S/C24H34F6O2/c1-3-5-7-8-9-10-12-14-19(13-11-6-4-2)32-22(31)20-17-18(23(25
InchiKey: MMKLLEUMGXPENO-UHFFFAOYSA-N
Formula: C24H34F6O2
SMILES: CCCCCCCCCC(CCCCC)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 468.52

Physical Properties

Property code	Value	Unit	Source
gf	-1155.19	kJ/mol	Joback Method
hf	-1769.34	kJ/mol	Joback Method
hfus	54.09	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	8.971		Crippen Method
mcvol	343.320	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	850.17	K	Joback Method
tc	1040.95	K	Joback Method
tf	477.24	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.53	J/mol×K	850.17	Joback Method
cpg	1130.07	J/mol×K	881.97	Joback Method
cpg	1146.54	J/mol×K	913.76	Joback Method
cpg	1162.00	J/mol×K	945.56	Joback Method
cpg	1176.52	J/mol×K	977.35	Joback Method
cpg	1190.16	J/mol×K	1009.15	Joback Method
cpg	1203.02	J/mol×K	1040.95	Joback Method

Sources

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=U338713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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