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

Inchi: InChI=1S/C17H20F6O2/c1-2-3-4-5-6-7-10-25-15(24)13-11-12(16(18,19)20)8-9-14(13)17
InchiKey: JHDIOKLRIOPDCI-UHFFFAOYSA-N
Formula: C17H20F6O2
SMILES: CCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 370.33

Physical Properties

Property code	Value	Unit	Source
gf	-1211.69	kJ/mol	Joback Method
hf	-1619.58	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	58.70	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.242		Crippen Method
mcvol	244.690	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	690.45	K	Joback Method
tc	864.25	K	Joback Method
tf	413.35	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.21	J/mol×K	690.45	Joback Method
cpg	720.83	J/mol×K	719.42	Joback Method
cpg	734.60	J/mol×K	748.38	Joback Method
cpg	747.56	J/mol×K	777.35	Joback Method
cpg	759.75	J/mol×K	806.31	Joback Method
cpg	771.22	J/mol×K	835.28	Joback Method
cpg	782.01	J/mol×K	864.25	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=U338941&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