Phthalic acid, octyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, octyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C24H27F3O4/c1-2-3-4-5-6-11-16-30-22(28)19-13-8-9-14-20(19)23(29)31-17-1
InchiKey: FGZGWOYHPATIGC-UHFFFAOYSA-N
Formula: C24H27F3O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 436.46

Physical Properties

Property code	Value	Unit	Source
gf	-692.67	kJ/mol	Joback Method
hf	-1175.25	kJ/mol	Joback Method
hfus	52.62	kJ/mol	Joback Method
hvap	89.46	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.580		Crippen Method
mcvol	321.690	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	959.00	K	Joback Method
tc	1176.98	K	Joback Method
tf	586.63	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.86	J/mol×K	959.00	Joback Method
cpg	1050.44	J/mol×K	995.33	Joback Method
cpg	1062.79	J/mol×K	1031.66	Joback Method
cpg	1073.99	J/mol×K	1067.99	Joback Method
cpg	1084.09	J/mol×K	1104.32	Joback Method
cpg	1093.16	J/mol×K	1140.65	Joback Method
cpg	1101.28	J/mol×K	1176.98	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=U377823&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