Decyl 2,3,4,5,6-pentafluorobenzoate

Other names: decyl pentafluorobenzoate
Inchi: InChI=1S/C17H21F5O2/c1-2-3-4-5-6-7-8-9-10-24-17(23)11-12(18)14(20)16(22)15(21)13
InchiKey: LXMRVZIXAUJRAE-UHFFFAOYSA-N
Formula: C17H21F5O2
SMILES: CCCCCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 352.34

Physical Properties

Property code	Value	Unit	Source
gf	-1051.45	kJ/mol	Joback Method
hf	-1440.38	kJ/mol	Joback Method
hfus	50.07	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.680		Crippen Method
mcvol	242.920	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2085.00		NIST Webbook
ripol	2082.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2089.00		NIST Webbook
tb	712.58	K	Joback Method
tc	883.70	K	Joback Method
tf	445.48	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.16	J/mol×K	712.58	Joback Method
cpg	706.44	J/mol×K	741.10	Joback Method
cpg	720.04	J/mol×K	769.62	Joback Method
cpg	732.95	J/mol×K	798.14	Joback Method
cpg	745.19	J/mol×K	826.66	Joback Method
cpg	756.76	J/mol×K	855.18	Joback Method
cpg	767.67	J/mol×K	883.70	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373599&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume