

1,2-Cyclohexanedicarboxylic acid, 2,5-dichlorophenyl heptyl ester

Inchi:	InChI=1S/C21H28Cl2O4/c1-2-3-4-5-8-13-26-20(24)16-9-6-7-10-17(16)21(25)27-19-14-15
InchiKey:	YCVKJHMWLMEMYMW-UHFFFAOYSA-N
Formula:	C21H28Cl2O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	415.35

Physical Properties

Property code	Value	Unit	Source
gf	-255.87	kJ/mol	Joback Method
hf	-750.28	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.219		Crippen Method
mvol	311.490	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	958.84	K	Joback Method
tc	1186.32	K	Joback Method
tf	585.19	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.46	J/molxK	958.84	Joback Method
cpg	1000.33	J/molxK	996.75	Joback Method
cpg	1012.58	J/molxK	1034.67	Joback Method
cpg	1023.23	J/molxK	1072.58	Joback Method
cpg	1032.31	J/molxK	1110.49	Joback Method
cpg	1039.85	J/molxK	1148.40	Joback Method
cpg	1045.88	J/molxK	1186.32	Joback Method
dvisc	0.0004012	Paxs	585.19	Joback Method

dvisc	0.0002381	Paxs	647.47	Joback Method
dvisc	0.0001548	Paxs	709.74	Joback Method
dvisc	0.0001079	Paxs	772.01	Joback Method
dvisc	0.0000794	Paxs	834.29	Joback Method
dvisc	0.0000610	Paxs	896.56	Joback Method
dvisc	0.0000484	Paxs	958.84	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=U339802&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
dvisc:	Dynamic viscosity
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

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