

Phenylacetic acid, 4-chloro-, heptadecyl ester

Inchi:	InChI=1S/C25H41ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-28-25(27)22-23-17
InchiKey:	SVDHLHUCKFAQBW-UHFFFAOYSA-N
Formula:	C25H41ClO2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	409.05

Physical Properties

Property code	Value	Unit	Source
gf	16.55	kJ/mol	Joback Method
hf	-594.81	kJ/mol	Joback Method
hfus	61.14	kJ/mol	Joback Method
hvap	87.72	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.297		Crippen Method
mvol	359.030	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	3099.00		NIST Webbook
rinpol	3099.00		NIST Webbook
tb	916.78	K	Joback Method
tc	1122.97	K	Joback Method
tf	512.53	K	Joback Method
vc	1.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.65	J/molxK	916.78	Joback Method
cpg	1241.25	J/molxK	1088.60	Joback Method
cpg	1227.40	J/molxK	1054.24	Joback Method
cpg	1212.48	J/molxK	1019.87	Joback Method
cpg	1196.41	J/molxK	985.51	Joback Method
cpg	1179.15	J/molxK	951.14	Joback Method
cpg	1254.08	J/molxK	1122.97	Joback Method
dvisc	0.0000320	Paxs	916.78	Joback Method

dvisc	0.0000422	Paxs	849.40	Joback Method
dvisc	0.0000583	Paxs	782.03	Joback Method
dvisc	0.0000856	Paxs	714.65	Joback Method
dvisc	0.0001362	Paxs	647.28	Joback Method
dvisc	0.0002412	Paxs	579.90	Joback Method
dvisc	0.0004967	Paxs	512.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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