

Benzamide, 2-chloro-N-(2-chlorobenzoyl)-N-(2-ethylhexyl)-

Inchi: InChI=1S/C22H25Cl2NO2/c1-3-5-10-16(4-2)15-25(21(26)17-11-6-8-13-19(17)23)22(27)1
InchiKey: IRGIEZZJKIVIQD-UHFFFAOYSA-N
Formula: C22H25Cl2NO2
SMILES: CCCCC(CC)CN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 406.35

Physical Properties

Property code	Value	Unit	Source
hfus	51.13	kJ/mol	Joback Method
log10ws	-6.59		Cheméo Relay (1.0)
logp	6.492		Crippen Method
mcvol	310.920	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	2811.00		NIST Webbook
rinpol	2811.00		NIST Webbook
tb	685.61	K	Cheméo Relay (1.0)
tf	317.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.83	J/mol×K	960.68	Joback Method
cpg	944.13	J/mol×K	999.36	Joback Method
cpg	956.37	J/mol×K	1038.04	Joback Method
cpg	967.65	J/mol×K	1076.72	Joback Method
cpg	978.06	J/mol×K	1115.40	Joback Method
cpg	987.71	J/mol×K	1154.09	Joback Method
cpg	996.70	J/mol×K	1192.77	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407500&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point

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