N,N'-[Methylenebis(2-chloro-4,1-phenylene)]bis(2,

Other names: Butyrylamide,
N,N'-[methylenebis(2-chloro-4,1-phenylene)]bis[2,2,3,3,4,4,4-heptafluoro-
N,N'-[methanediylbis(2-chlorobenzene-4,1-diyl)]bis(2,2,3,3,4,4,4-heptafluorobutyrylamide
N-[2-Chloro-4-[[3-chloro-4-[(2,2,3,3,4,4,4-heptafluorobutyryl)amino]phenyl]methyl]phenyl]-

Inchi: InChI=1S/C21H10Cl2F14N2O2/c22-10-6-8(1-3-12(10)38-14(40)16(24,25)18(28,29)20(32

InchiKey: FTWLUZZOWSUZJK-UHFFFAOYSA-N

Formula: C21H10Cl2F14N2O2

SMILES: O=C(Nc1ccc(Cc2ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(Cl)c2)cc1Cl)C(F)(F)C(F)(F)C(F)(F

Mol. weight [g/mol]: 659.20

Physical Properties

Property code	Value	Unit	Source
gf	-2500.98	kJ/mol	Joback Method
hf	-2997.33	kJ/mol	Joback Method
hfus	57.10	kJ/mol	Joback Method
hvap	85.46	kJ/mol	Joback Method
log10ws	-9.60		Crippen Method
logp	8.127		Crippen Method
mcvol	331.590	ml/mol	McGowan Method
pc	1061.02	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	1006.50	K	Joback Method
tc	1233.04	K	Joback Method
tf	717.15	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.29	J/mol×K	1006.50	Joback Method
cpg	1040.49	J/mol×K	1044.26	Joback Method
cpg	1049.65	J/mol×K	1082.01	Joback Method
cpg	1059.00	J/mol×K	1119.77	Joback Method
cpg	1068.77	J/mol×K	1157.52	Joback Method

cpg	1079.19	J/mol×K	1195.28	Joback Method
cpg	1090.50	J/mol×K	1233.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373300&Units=SI

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

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